Sample name: **M12_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03014**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03014_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 6:11:21 PM**
Analyst: **Pion**
Instrument ID: **T312060**

pH-metric Result

logP (XH +) 0.62 ±0.05 (n=50)
logP (neutral X) 3.91 ±0.01 (n=50)

18C-03014 Points 1 to 25

M12_octanol concentration factor 0.960
Carbonate 0.5327 mM
Acidity error -1.77424 mM

18C-03014 Points 26 to 51

M12_octanol concentration factor 1.007
Carbonate 0.2455 mM
Acidity error -1.88168 mM

18C-03014 Points 52 to 76

M12_octanol concentration factor 1.171
Carbonate 0.3091 mM
Acidity error -3.49881 mM

Warnings and errors

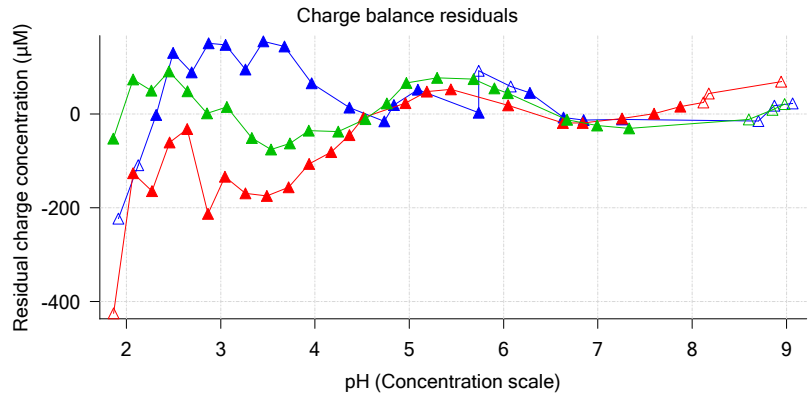
Errors None
Warnings Excessive carbonate concentration present

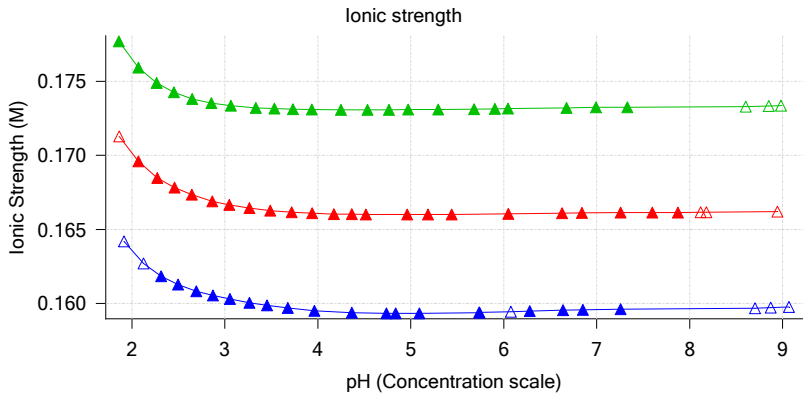
Sample logD and percent species

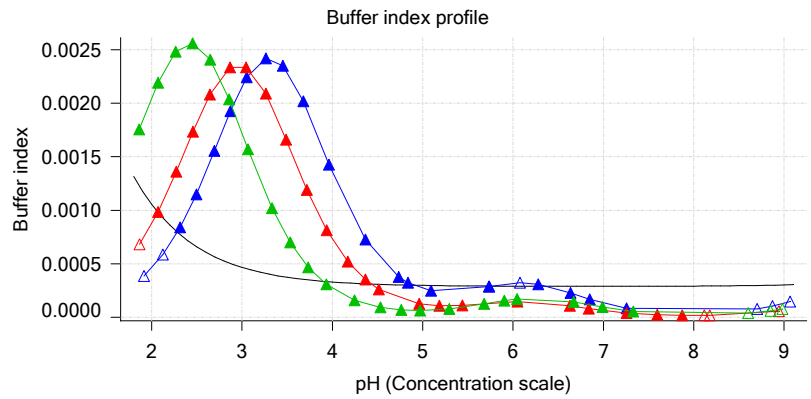
pH	M12_octanol logD	M12_octanol M12_octanolH	M12_octanol M12_octanol	M12_octanol M12_octanolH*	M12_octanol M12_octanol*	Comment
1.000	0.66	17.81 %	0.00 %	74.63 %	7.56 %	
1.200	0.69	17.06 %	0.00 %	71.47 %	11.47 %	Stomach pH
2.000	0.93	10.60 %	0.01 %	44.41 %	44.98 %	
3.000	1.67	2.10 %	0.01 %	8.80 %	89.09 %	
4.000	2.61	0.23 %	0.01 %	0.98 %	98.78 %	
5.000	3.45	0.02 %	0.01 %	0.10 %	99.87 %	
6.000	3.83	0.00 %	0.01 %	0.01 %	99.98 %	
6.500	3.88	0.00 %	0.01 %	0.00 %	99.98 %	
7.000	3.90	0.00 %	0.01 %	0.00 %	99.99 %	
7.400	3.90	0.00 %	0.01 %	0.00 %	99.99 %	Blood pH
8.000	3.91	0.00 %	0.01 %	0.00 %	99.99 %	
9.000	3.91	0.00 %	0.01 %	0.00 %	99.99 %	
10.000	3.91	0.00 %	0.01 %	0.00 %	99.99 %	
11.000	3.91	0.00 %	0.01 %	0.00 %	99.99 %	
12.000	3.91	0.00 %	0.01 %	0.00 %	99.99 %	

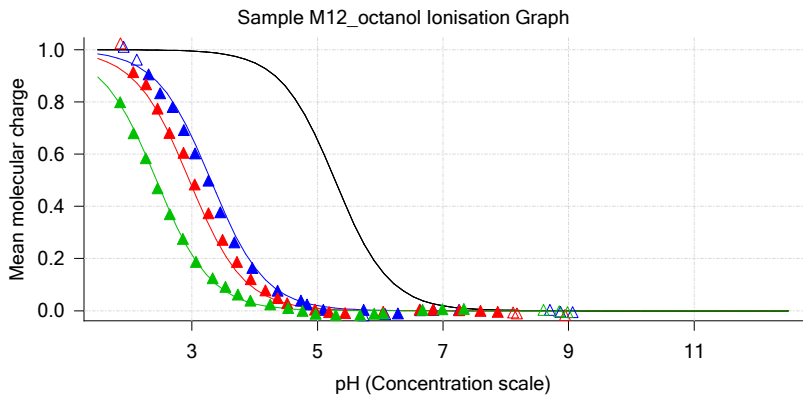
Sample name:	**M12_octanol**	Experiment start time:	**3/3/2018 6:11:21 PM**
Assay name:	**pH-metric high logP**	Analyst:	**Pion**
Assay ID:	**18C-03014**	Instrument ID:	**T312060**
Filename:	**C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03014_M12_octanol_pH-metric high logP.t3r**		

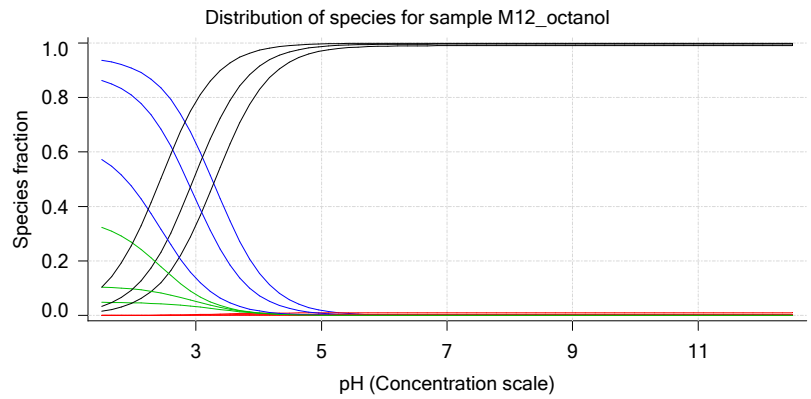
Graphs

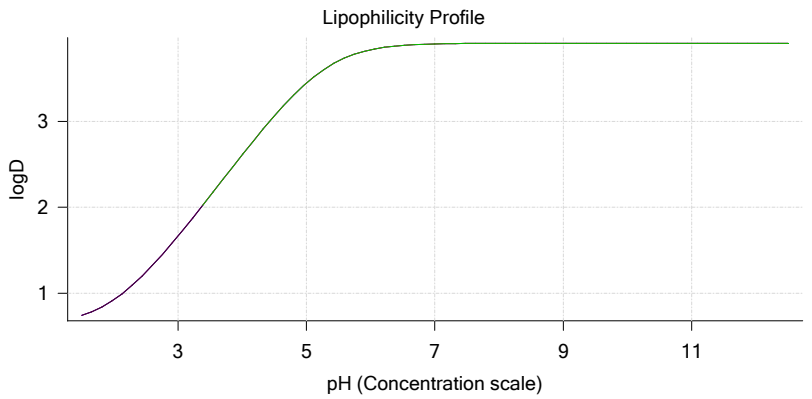


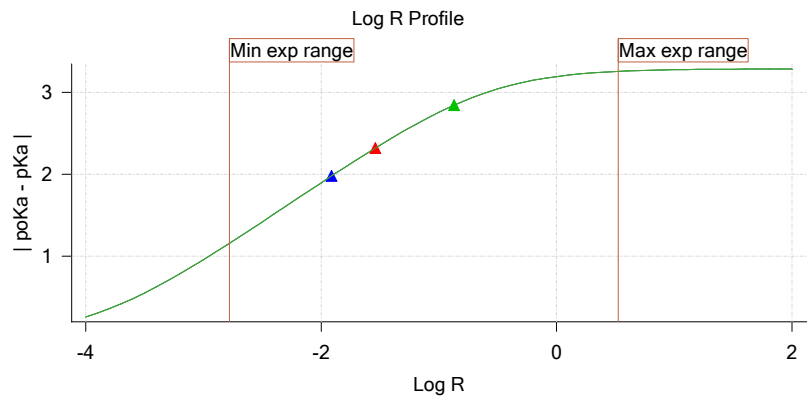


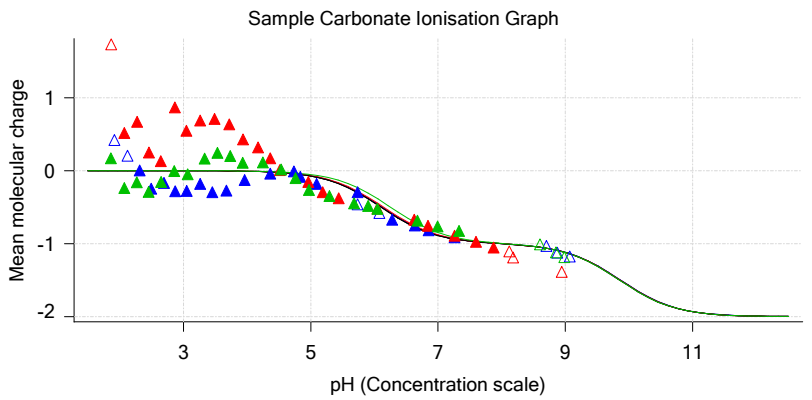








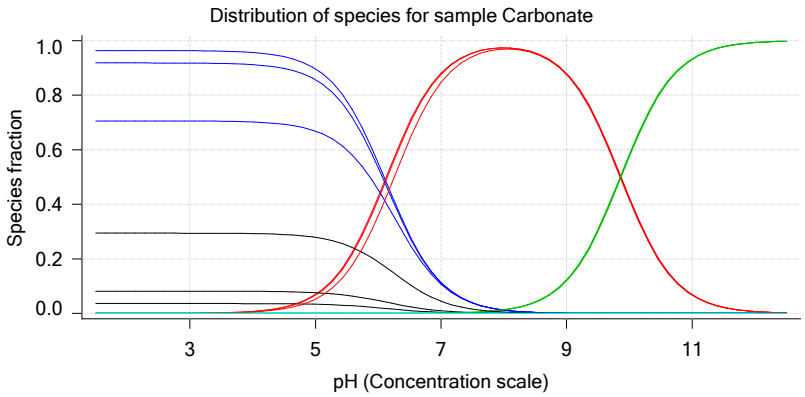




Sample name: **M12_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03014**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03014_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 6:11:21 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Graphs (continued)



Sample name:	**M12_octanol**	Experiment start time:	**3/3/2018 6:11:21 PM**
Assay name:	**pH-metric high logP**	Analyst:	**Pion**
Assay ID:	**18C-03014**	Instrument ID:	**T312060**
Filename:	**C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03014_M12_octanol_pH-metric high logP.t3r**		

pH-metric high logP Titration 1 of 3 18C-03014 Points 1 to 25

Overall results

RMSD	0.070
Average ionic strength	0.160 M
Average temperature	24.9°C
Partition ratio	0.0123 : 1
Analyte concentration range	4301.0 µM to 4446.8 µM
Total points considered	18 of 25

Warnings and errors

Errors	None
Warnings	Excessive carbonate concentration present
	Excessive acidity error present

Four-Plus parameters

Alpha	0.111	3/3/2018 6:11:21 PM	C:\Sirius_T3\HCl18C02.t3r
S	0.9988	3/3/2018 6:11:21 PM	C:\Sirius_T3\HCl18C02.t3r
jH	1.0	3/3/2018 6:11:21 PM	C:\Sirius_T3\HCl18C02.t3r
jOH	-0.8	3/3/2018 6:11:21 PM	C:\Sirius_T3\HCl18C02.t3r

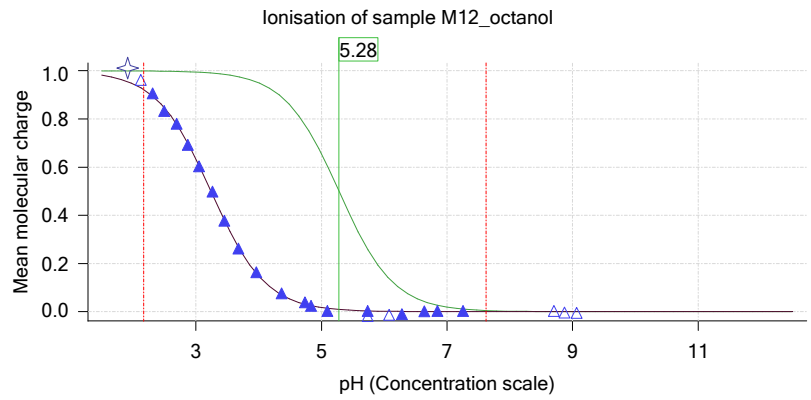
Titrants

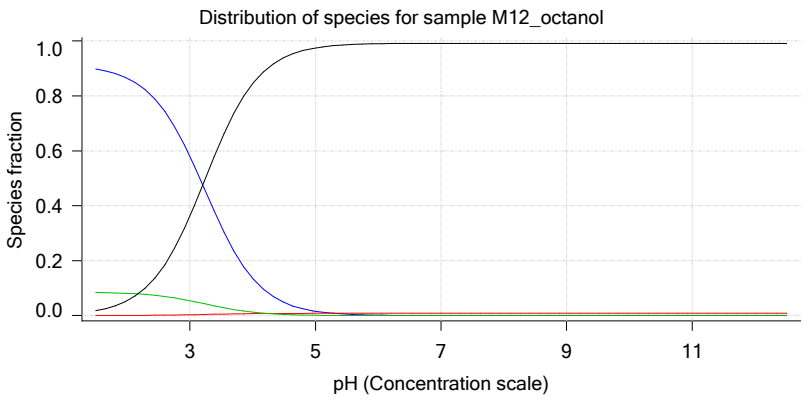
0.50 M HCl	0.999058	3/3/2018 6:11:21 PM	C:\Sirius_T3\HCl18C02.t3r
0.50 M KOH	0.999845	3/3/2018 6:11:21 PM	C:\Sirius_T3\KOH18B27.t3r

Sample

M12_octanol concentration factor	0.960
M12_octanol stoichiometry	1.000
Chloride stoichiometry	1.000
Base pKa 1	5.28
logP (XH +)	0.88
logP (neutral X)	3.99

Sample graphs

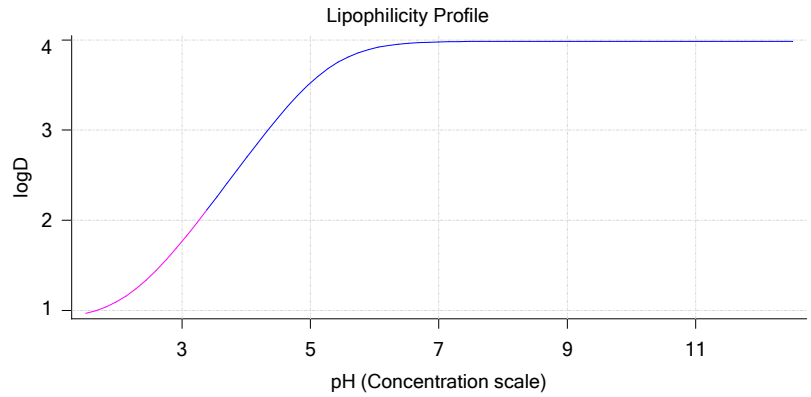




Sample name: **M12_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03014**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03014_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 6:11:21 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Sample graphs (continued)



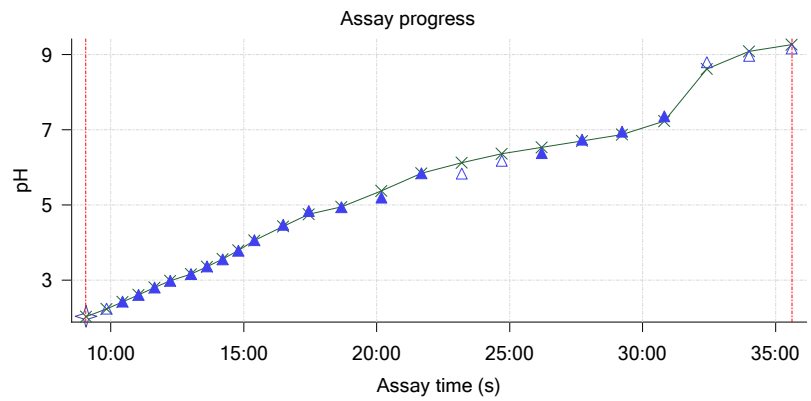
Sample logD and percent species

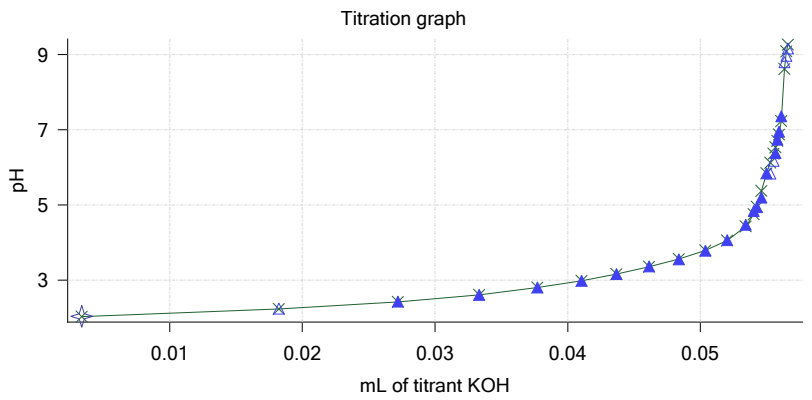
pH	M12_octanol logD	M12_octanol M12_octanolH	M12_octanol M12_octanol	M12_octanol M12_octanolH*	M12_octanol M12_octanol*	Comment
1.000	0.91	90.92 %	0.00 %	8.51 %	0.57 %	
1.200	0.93	90.62 %	0.01 %	8.48 %	0.90 %	Stomach pH
2.000	1.10	86.47 %	0.05 %	8.09 %	5.39 %	
3.000	1.76	58.05 %	0.30 %	5.43 %	36.21 %	
4.000	2.69	13.54 %	0.71 %	1.27 %	84.48 %	
5.000	3.52	1.56 %	0.82 %	0.15 %	97.47 %	
6.000	3.91	0.16 %	0.83 %	0.01 %	98.99 %	
6.500	3.96	0.05 %	0.83 %	0.00 %	99.11 %	
7.000	3.98	0.02 %	0.83 %	0.00 %	99.15 %	
7.400	3.98	0.01 %	0.83 %	0.00 %	99.16 %	Blood pH
8.000	3.99	0.00 %	0.83 %	0.00 %	99.16 %	
9.000	3.99	0.00 %	0.83 %	0.00 %	99.17 %	
10.000	3.99	0.00 %	0.83 %	0.00 %	99.17 %	
11.000	3.99	0.00 %	0.83 %	0.00 %	99.17 %	
12.000	3.99	0.00 %	0.83 %	0.00 %	99.17 %	

Carbonate and acidity

Carbonate 0.533 mM
Acidity error -1.774 mM

Other graphs

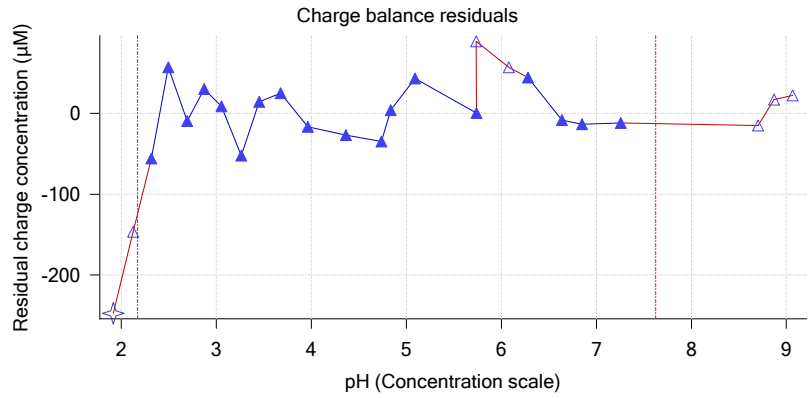


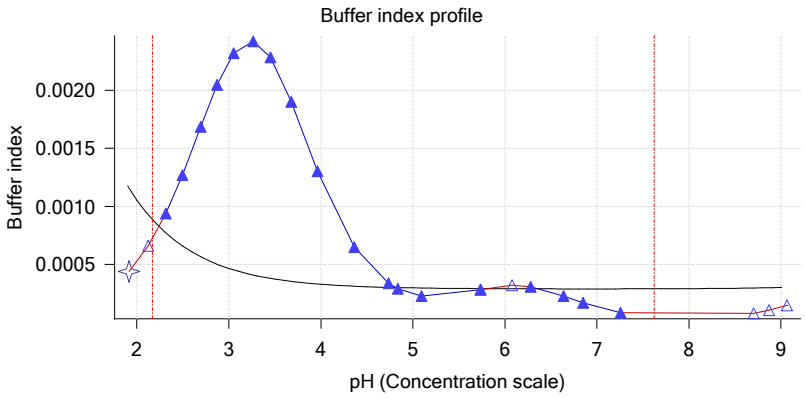


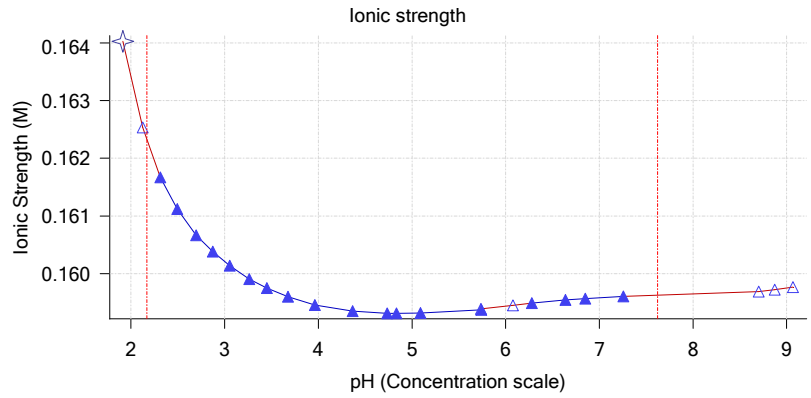
Sample name: **M12_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03014**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03014_M12_octanol_pH-metric high logP.t3r**

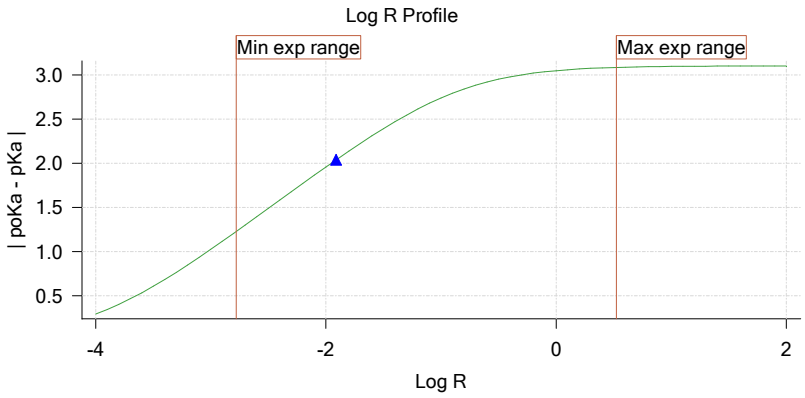
Experiment start time: **3/3/2018 6:11:21 PM**
Analyst: **Pion**
Instrument ID: **T312060**

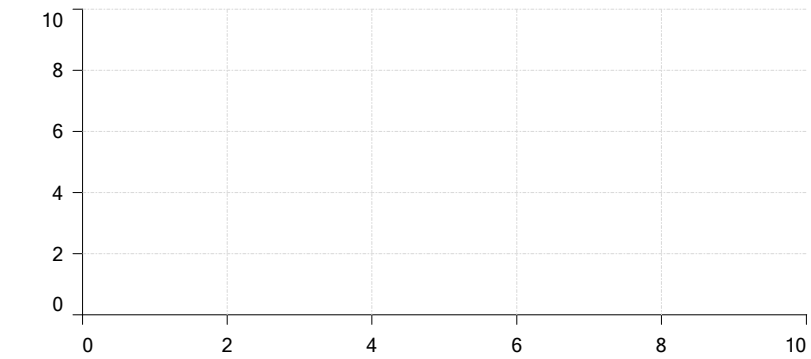
Other graphs (continued)

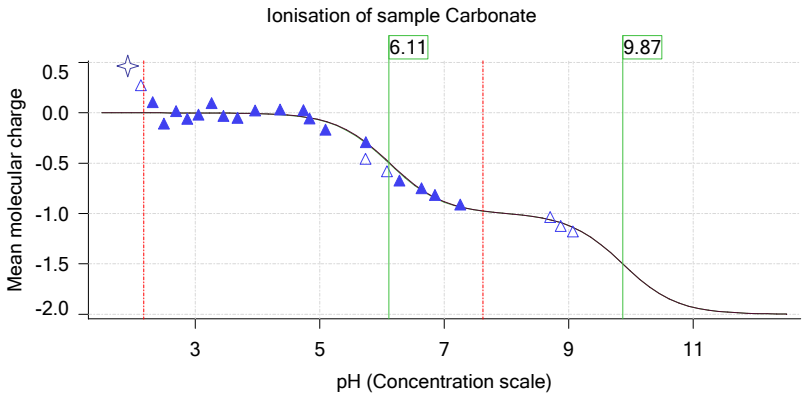












Sample name:	**M12_octanol**	Experiment start time:	**3/3/2018 6:11:21 PM**
Assay name:	**pH-metric high logP**	Analyst:	**Pion**
Assay ID:	**18C-03014**	Instrument ID:	**T312060**
Filename:	**C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03014_M12_octanol_pH-metric high logP.t3r**		

pH-metric high logP Titration 2 of 3 18C-03014 Points 26 to 51

Overall results

RMSD	0.236
Average ionic strength	0.166 M
Average temperature	25.0°C
Partition ratio	0.0288 : 1
Analyte concentration range	3930.3 µM to 4070.1 µM
Total points considered	22 of 26

Warnings and errors

Errors	None
Warnings	Excessive acidity error present

Four-Plus parameters

Alpha	0.111	3/3/2018 6:11:21 PM	C:\Sirius_T3\HCl18C02.t3r
S	0.9988	3/3/2018 6:11:21 PM	C:\Sirius_T3\HCl18C02.t3r
jH	1.0	3/3/2018 6:11:21 PM	C:\Sirius_T3\HCl18C02.t3r
jOH	-0.8	3/3/2018 6:11:21 PM	C:\Sirius_T3\HCl18C02.t3r

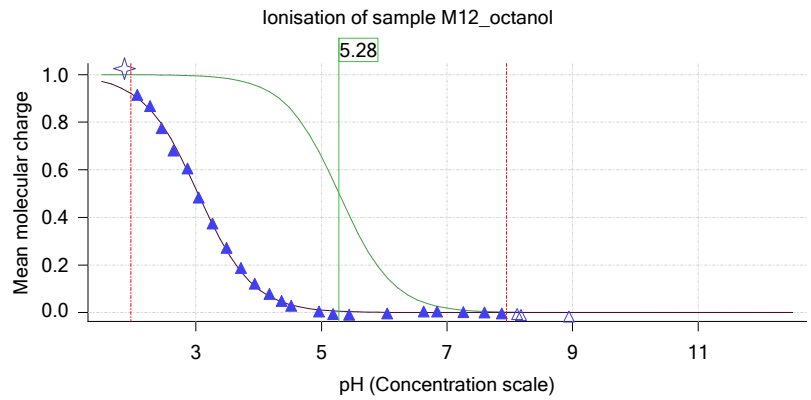
Titrants

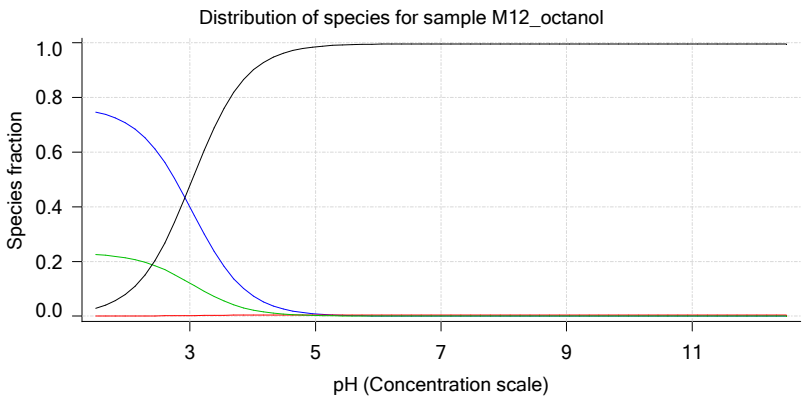
0.50 M HCl	0.999058	3/3/2018 6:11:21 PM	C:\Sirius_T3\HCl18C02.t3r
0.50 M KOH	0.999845	3/3/2018 6:11:21 PM	C:\Sirius_T3\KOH18B27.t3r

Sample

M12_octanol concentration factor	1.007
M12_octanol stoichiometry	1.000
Chloride stoichiometry	1.000
Base pKa 1	5.28
logP (XH +)	1.02
logP (neutral X)	3.90

Sample graphs

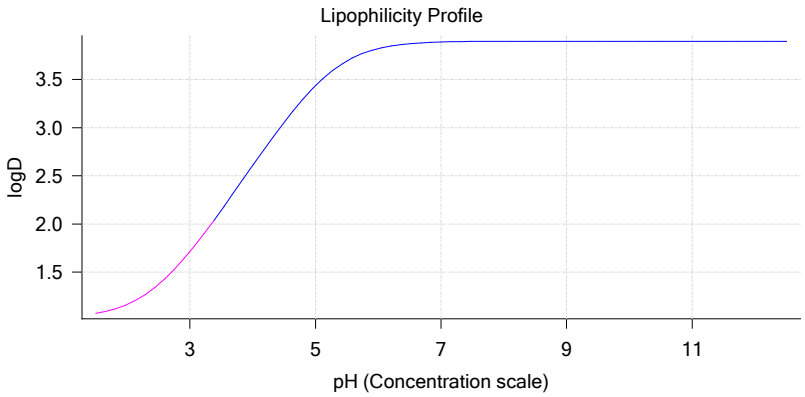




Sample name: **M12_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03014**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03014_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 6:11:21 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Sample graphs (continued)



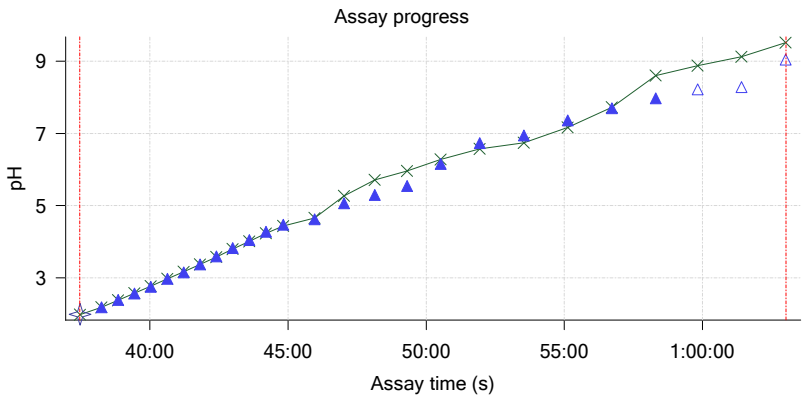
Sample logD and percent species

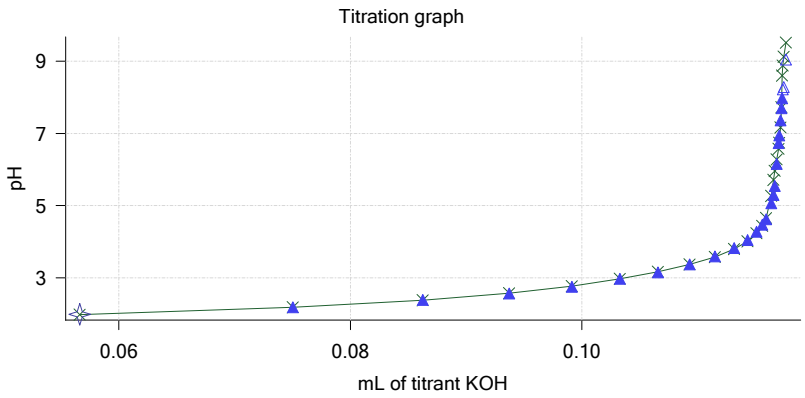
pH	M12_octanol logD	M12_octanol M12_octanolH	M12_octanol M12_octanol	M12_octanol M12_octanolH*	M12_octanol M12_octanol*	Comment
1.000	1.04	76.11 %	0.00 %	22.98 %	0.91 %	
1.200	1.05	75.71 %	0.01 %	22.85 %	1.43 %	Stomach pH
2.000	1.16	70.33 %	0.04 %	21.23 %	8.40 %	
3.000	1.71	39.98 %	0.21 %	12.07 %	47.74 %	
4.000	2.61	7.52 %	0.39 %	2.27 %	89.81 %	
5.000	3.44	0.82 %	0.43 %	0.25 %	98.49 %	
6.000	3.82	0.08 %	0.44 %	0.03 %	99.45 %	
6.500	3.87	0.03 %	0.44 %	0.01 %	99.53 %	
7.000	3.89	0.01 %	0.44 %	0.00 %	99.55 %	
7.400	3.89	0.00 %	0.44 %	0.00 %	99.56 %	Blood pH
8.000	3.90	0.00 %	0.44 %	0.00 %	99.56 %	
9.000	3.90	0.00 %	0.44 %	0.00 %	99.56 %	
10.000	3.90	0.00 %	0.44 %	0.00 %	99.56 %	
11.000	3.90	0.00 %	0.44 %	0.00 %	99.56 %	
12.000	3.90	0.00 %	0.44 %	0.00 %	99.56 %	

Carbonate and acidity

Carbonate 0.246 mM
Acidity error -1.882 mM

Other graphs

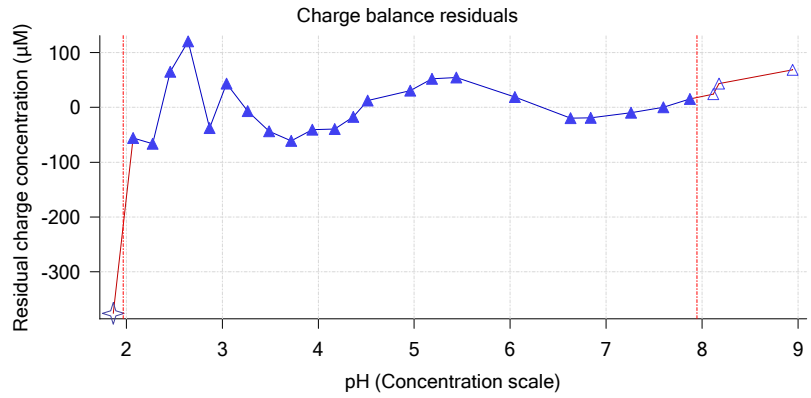


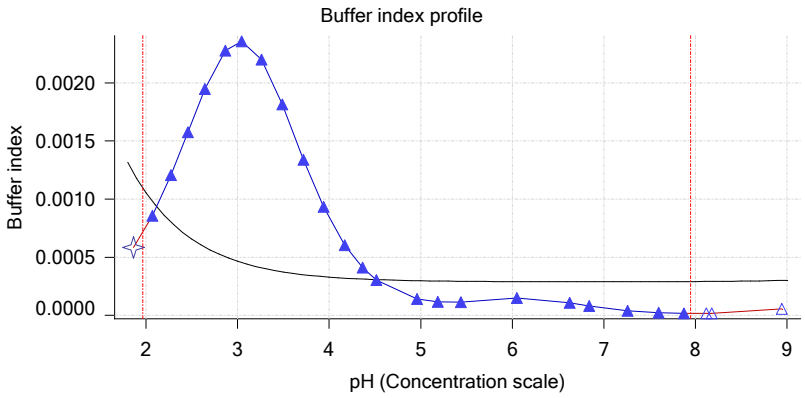


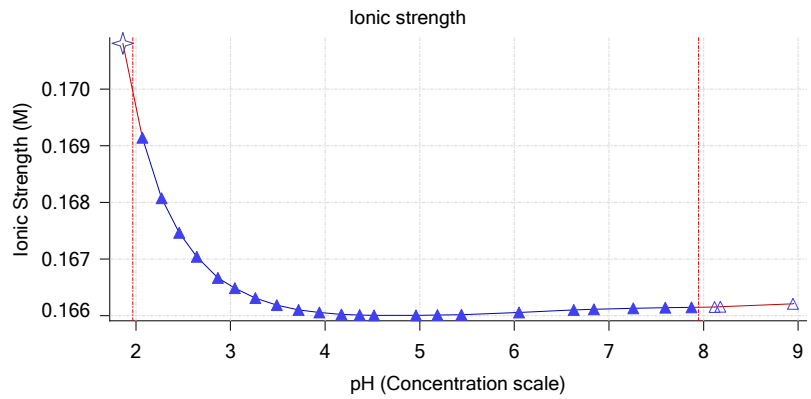
Sample name: **M12_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03014**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03014_M12_octanol_pH-metric high logP.t3r**

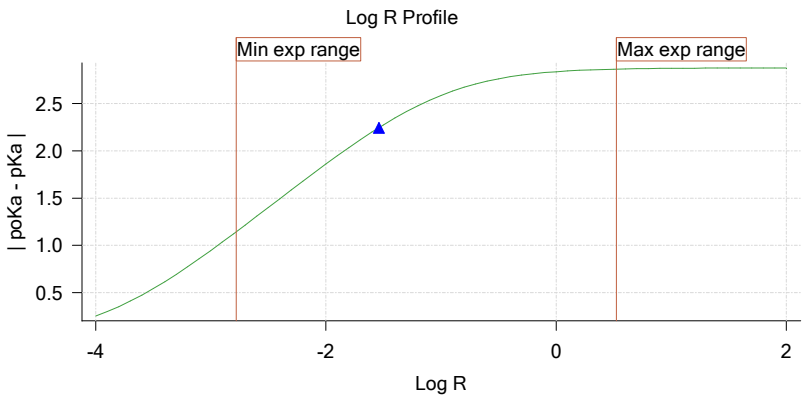
Experiment start time: **3/3/2018 6:11:21 PM**
Analyst: **Pion**
Instrument ID: **T312060**

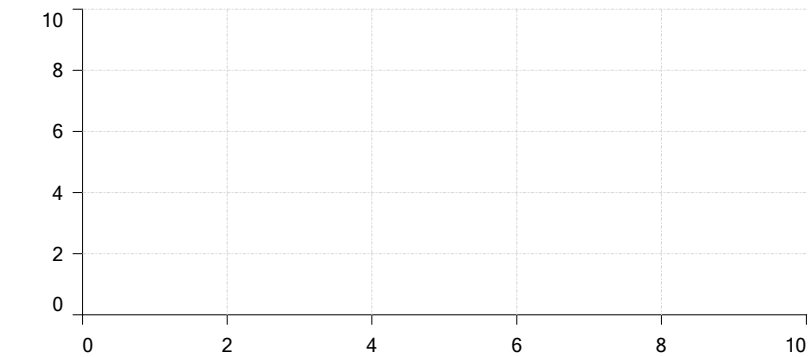
Other graphs (continued)

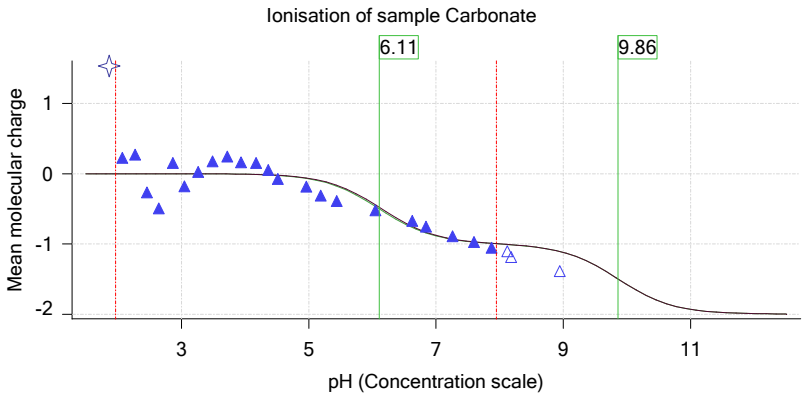












Sample name:	**M12_octanol**	Experiment start time:	**3/3/2018 6:11:21 PM**
Assay name:	**pH-metric high logP**	Analyst:	**Pion**
Assay ID:	**18C-03014**	Instrument ID:	**T312060**
Filename:	**C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03014_M12_octanol_pH-metric high logP.t3r**		

pH-metric high logP Titration 3 of 3 18C-03014 Points 52 to 76

Overall results

RMSD	0.325
Average ionic strength	0.174 M
Average temperature	25.0°C
Partition ratio	0.1350 : 1
Analyte concentration range	3312.8 µM to 3415.8 µM
Total points considered	22 of 25

Warnings and errors

Errors	None
Warnings	Excessive acidity error present

Four-Plus parameters

Alpha	0.111	3/3/2018 6:11:21 PM	C:\Sirius_T3\HCl18C02.t3r
S	0.9988	3/3/2018 6:11:21 PM	C:\Sirius_T3\HCl18C02.t3r
jH	1.0	3/3/2018 6:11:21 PM	C:\Sirius_T3\HCl18C02.t3r
jOH	-0.8	3/3/2018 6:11:21 PM	C:\Sirius_T3\HCl18C02.t3r

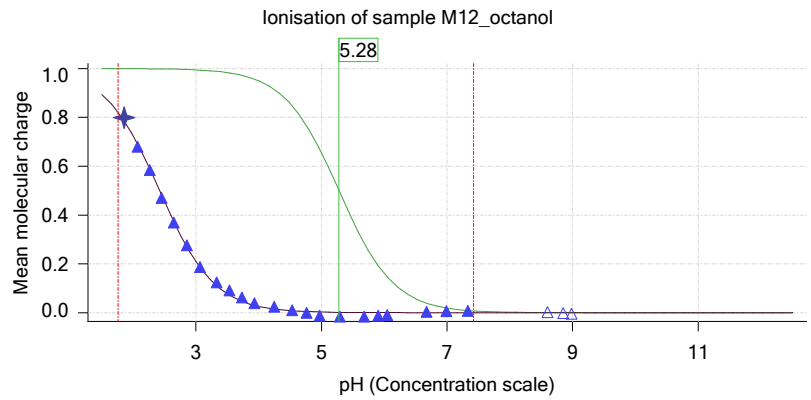
Titrants

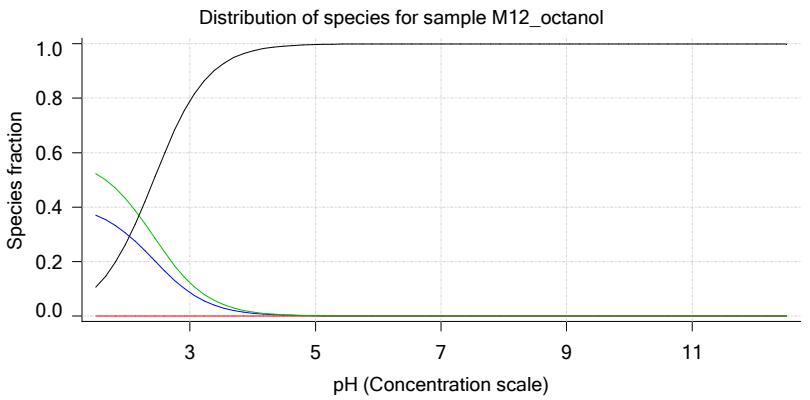
0.50 M HCl	0.999058	3/3/2018 6:11:21 PM	C:\Sirius_T3\HCl18C02.t3r
0.50 M KOH	0.999845	3/3/2018 6:11:21 PM	C:\Sirius_T3\KOH18B27.t3r

Sample

M12_octanol concentration factor	1.171
M12_octanol stoichiometry	1.000
Chloride stoichiometry	1.000
Base pKa 1	5.28
logP (XH +)	1.02
logP (neutral X)	4.11

Sample graphs

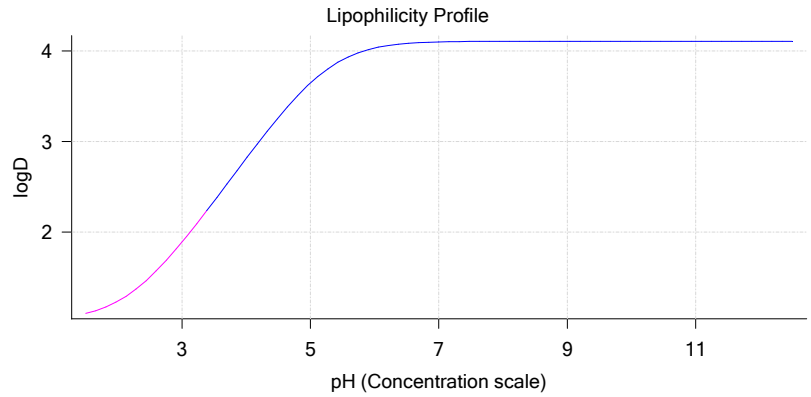




Sample name: **M12_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03014**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03014_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 6:11:21 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Sample graphs (continued)



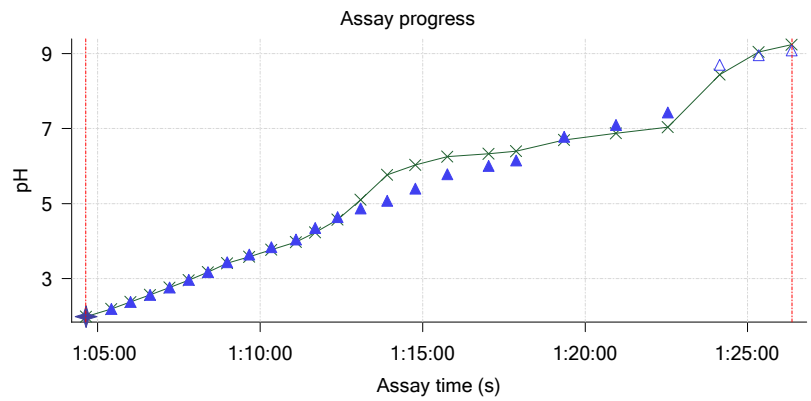
Sample logD and percent species

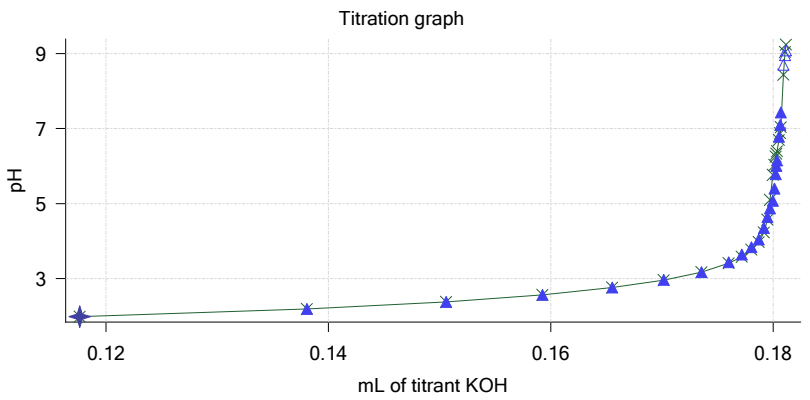
pH	M12_octanol logD	M12_octanol M12_octanolH	M12_octanol M12_octanol	M12_octanol M12_octanolH*	M12_octanol M12_octanol*	Comment
1.000	1.05	39.92 %	0.00 %	56.44 %	3.63 %	
1.200	1.06	39.09 %	0.00 %	55.27 %	5.64 %	Stomach pH
2.000	1.24	30.08 %	0.02 %	42.52 %	27.38 %	
3.000	1.89	8.68 %	0.05 %	12.27 %	79.01 %	
4.000	2.81	1.07 %	0.06 %	1.51 %	97.36 %	
5.000	3.65	0.11 %	0.06 %	0.15 %	99.68 %	
6.000	4.03	0.01 %	0.06 %	0.02 %	99.92 %	
6.500	4.08	0.00 %	0.06 %	0.00 %	99.93 %	
7.000	4.10	0.00 %	0.06 %	0.00 %	99.94 %	
7.400	4.11	0.00 %	0.06 %	0.00 %	99.94 %	Blood pH
8.000	4.11	0.00 %	0.06 %	0.00 %	99.94 %	
9.000	4.11	0.00 %	0.06 %	0.00 %	99.94 %	
10.000	4.11	0.00 %	0.06 %	0.00 %	99.94 %	
11.000	4.11	0.00 %	0.06 %	0.00 %	99.94 %	
12.000	4.11	0.00 %	0.06 %	0.00 %	99.94 %	

Carbonate and acidity

Carbonate 0.309 mM
Acidity error -3.499 mM

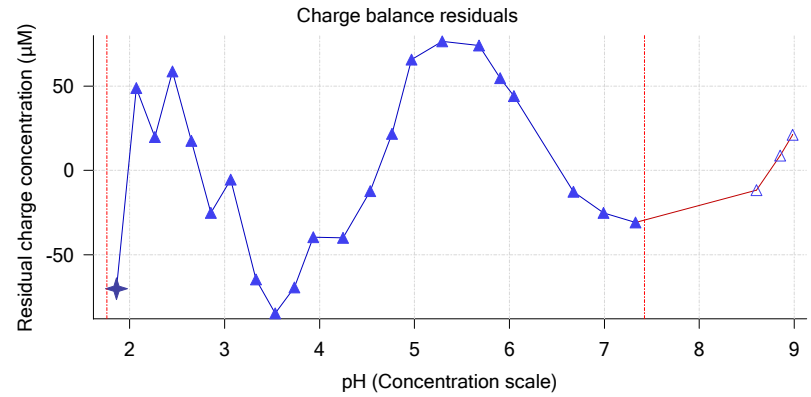
Other graphs

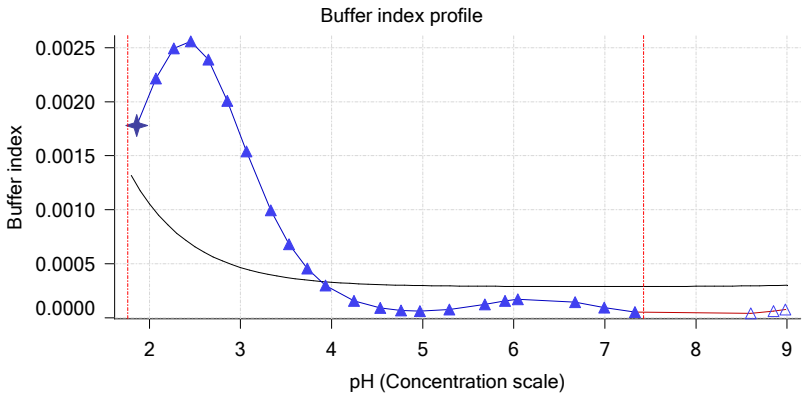


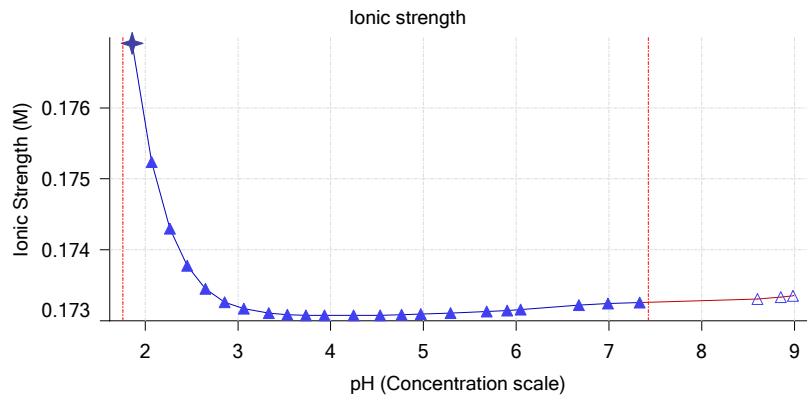


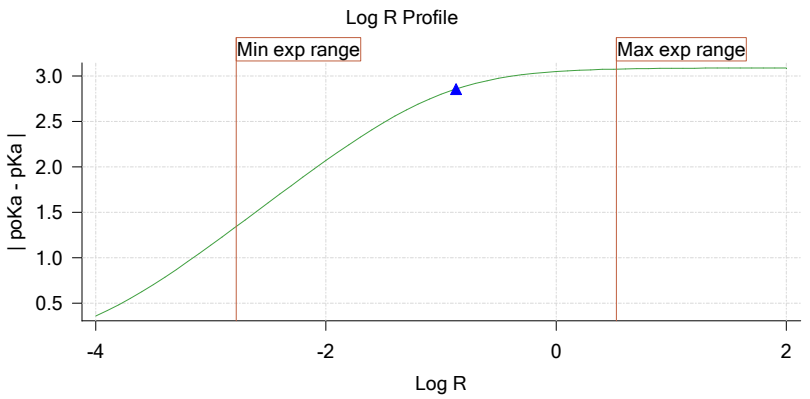
Sample name:	**M12_octanol**	Experiment start time:	**3/3/2018 6:11:21 PM**
Assay name:	**pH-metric high logP**	Analyst:	**Pion**
Assay ID:	**18C-03014**	Instrument ID:	**T312060**
Filename:	**C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03014_M12_octanol_pH-metric high logP.t3r**		

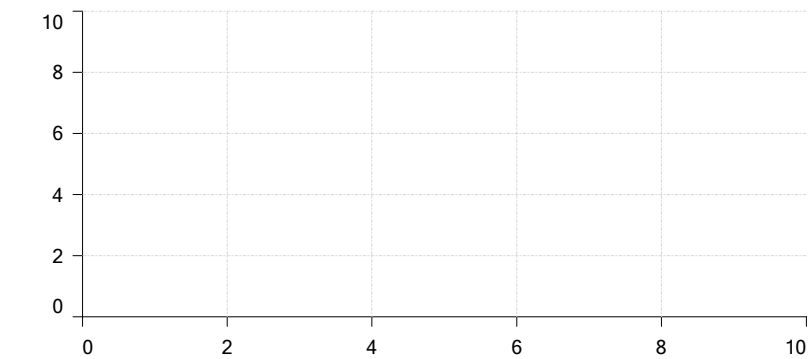
Other graphs (continued)

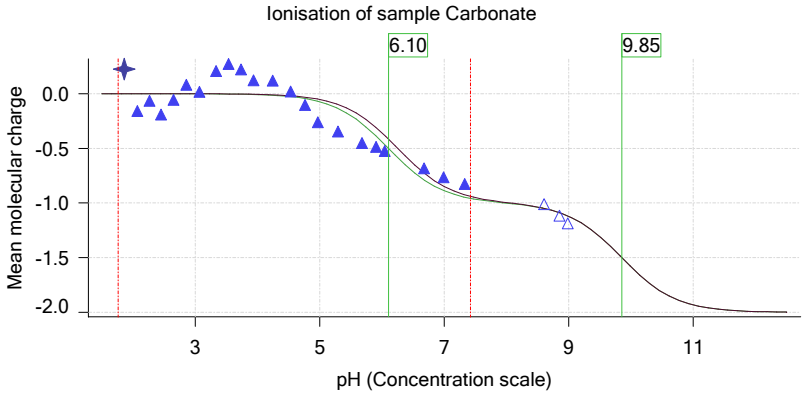












Sample name: **M12_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03014**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03014_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 6:11:21 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	M12_octanol	2/28/2018 2:58:36 PM	User entered value
Sample by	Weight		Default value
Sample weight	0.002040 g	3/2/2018 5:10:25 PM	User entered value
Formula weight	292.16 g/mol	2/28/2018 2:58:36 PM	User entered value
Solubility	Unknown		Default value
Molecular weight	255.70	2/28/2018 2:58:36 PM	User entered value
Individual pKa ionic environments	No		Default value
Number of pKas	1	2/28/2018 2:58:36 PM	User entered value
Sample is a	Base	2/28/2018 2:58:36 PM	User entered value
pKa 1	5.28	2/28/2018 2:58:36 PM	User entered value
logp (XH +)	1.02	3/2/2018 3:44:28 PM	User entered value
logP (neutral X)	3.79	3/2/2018 3:44:35 PM	User entered value
Stoichiometry	1.00000		Default value
Aprotic counterion name	Chloride		From standards.xml file
Stoichiometry	1.00		From standards.xml file
Charge per counterion	-1		From standards.xml file

Events

Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
5:59.7	Initial pH = 3.54									
9:04.2	Data point 1	1.50000 mL	0.04685 mL	0.00336 mL	0.01999 mL	2.035	-0.01024	0.61219	0.00065	10.0 s
9:50.4	Data point 2	1.50000 mL	0.04685 mL	0.01823 mL	0.01999 mL	2.240	-0.00195	0.36606	0.00016	10.5 s
10:26.5	Data point 3	1.50000 mL	0.04685 mL	0.02721 mL	0.01999 mL	2.427	-0.00750	0.72499	0.00043	10.5 s
11:02.6	Data point 4	1.50000 mL	0.04685 mL	0.03333 mL	0.01999 mL	2.606	-0.00567	0.86217	0.00030	10.5 s
11:38.7	Data point 5	1.50000 mL	0.04685 mL	0.03772 mL	0.01999 mL	2.803	-0.01366	0.90570	0.00071	10.0 s
12:14.2	Data point 6	1.50000 mL	0.04685 mL	0.04104 mL	0.01999 mL	2.980	-0.01014	0.26097	0.00098	11.0 s
13:01.1	Data point 7	1.50000 mL	0.04685 mL	0.04367 mL	0.01999 mL	3.161	-0.00882	0.80998	0.00048	10.5 s
13:37.0	Data point 8	1.50000 mL	0.04685 mL	0.04614 mL	0.01999 mL	3.370	-0.00523	0.34459	0.00044	10.0 s
14:12.5	Data point 9	1.50000 mL	0.04685 mL	0.04838 mL	0.01999 mL	3.558	-0.00999	0.44733	0.00074	10.0 s
14:48.0	Data point 10	1.50000 mL	0.04685 mL	0.05038 mL	0.01999 mL	3.784	-0.01707	0.81320	0.00094	10.5 s
15:24.0	Data point 11	1.50000 mL	0.04685 mL	0.05202 mL	0.01999 mL	4.069	-0.01895	0.92370	0.00097	29.5 s
16:29.4	Data point 12	1.50000 mL	0.04685 mL	0.05341 mL	0.01999 mL	4.470	-0.01716	0.79592	0.00095	22.0 s
17:27.1	Data point 13	1.50000 mL	0.04685 mL	0.05402 mL	0.01999 mL	4.841	-0.01868	0.91616	0.00096	47.5 s
18:40.1	Data point 14	1.50000 mL	0.04685 mL	0.05426 mL	0.01999 mL	4.941	-0.02276	0.93191	0.00116	Timed out at 59.5 s
20:10.6	Data point 15	1.50000 mL	0.04685 mL	0.05461 mL	0.01999 mL	5.196	-0.04657	0.99269	0.00231	Timed out at 59.5 s
21:41.2	Data point 16	1.50000 mL	0.04685 mL	0.05499 mL	0.01999 mL	5.842	-0.13692	0.98959	0.00680	Timed out at 59.5 s
23:11.7	Data point 17	1.50000 mL	0.04685 mL	0.05527 mL	0.01999 mL	5.839	-0.10548	0.98431	0.00525	Timed out at 59.5 s
24:42.2	Data point 18	1.50000 mL	0.04685 mL	0.05550 mL	0.01999 mL	6.181	-0.07455	0.99489	0.00369	Timed out at 59.5 s
26:12.7	Data point 19	1.50000 mL	0.04685 mL	0.05567 mL	0.01999 mL	6.383	-0.02576	0.98099	0.00128	Timed out at 59.5 s
27:43.2	Data point 20	1.50000 mL	0.04685 mL	0.05581 mL	0.01999 mL	6.739	-0.03694	0.97684	0.00185	Timed out at 59.5 s
29:13.6	Data point 21	1.50000 mL	0.04685 mL	0.05593 mL	0.01999 mL	6.952	-0.03900	0.97414	0.00195	Timed out at 59.5 s
30:49.3	Data point 22	1.50000 mL	0.04685 mL	0.05609 mL	0.01999 mL	7.359	-0.06446	0.99560	0.00319	Timed out at 59.5 s
32:25.0	Data point 23	1.50000 mL	0.04685 mL	0.05633 mL	0.01999 mL	8.802	-0.02839	0.97337	0.00142	Timed out at 59.5 s
34:00.7	Data point 24	1.50000 mL	0.04685 mL	0.05649 mL	0.01999 mL	8.971	-0.03345	0.98026	0.00167	Timed out at 59.5 s
35:36.4	Data point 25	1.50000 mL	0.04685 mL	0.05661 mL	0.01999 mL	9.166	-0.01865	0.93346	0.00095	48.0 s

Sample name: **M12_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03014**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03014_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 6:11:21 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Events (continued)

Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
37:28.6	Data point 26	1.50000 mL	0.10894 mL	0.05661 mL	0.05000 mL	1.986	-0.01183	0.86781	0.00063	10.0 s
38:14.8	Data point 27	1.50000 mL	0.10894 mL	0.07502 mL	0.05000 mL	2.187	-0.01196	0.55172	0.00080	10.5 s
38:51.0	Data point 28	1.50000 mL	0.10894 mL	0.08624 mL	0.05000 mL	2.386	-0.00645	0.60653	0.00041	10.0 s
39:26.5	Data point 29	1.50000 mL	0.10894 mL	0.09372 mL	0.05000 mL	2.568	-0.00151	0.03213	0.00042	10.0 s
40:02.1	Data point 30	1.50000 mL	0.10894 mL	0.09913 mL	0.05000 mL	2.753	-0.00324	0.58318	0.00021	10.5 s
40:38.2	Data point 31	1.50000 mL	0.10894 mL	0.10329 mL	0.05000 mL	2.974	-0.00350	0.62117	0.00022	10.0 s
41:13.7	Data point 32	1.50000 mL	0.10894 mL	0.10656 mL	0.05000 mL	3.153	-0.00315	0.45340	0.00023	10.0 s
41:49.2	Data point 33	1.50000 mL	0.10894 mL	0.10931 mL	0.05000 mL	3.370	-0.00431	0.37822	0.00035	10.0 s
42:24.7	Data point 34	1.50000 mL	0.10894 mL	0.11150 mL	0.05000 mL	3.595	-0.01024	0.34800	0.00086	10.0 s
43:00.1	Data point 35	1.50000 mL	0.10894 mL	0.11315 mL	0.05000 mL	3.826	-0.01287	0.75168	0.00073	10.5 s
43:36.1	Data point 36	1.50000 mL	0.10894 mL	0.11432 mL	0.05000 mL	4.044	-0.01264	0.72037	0.00074	11.0 s
44:12.5	Data point 37	1.50000 mL	0.10894 mL	0.11510 mL	0.05000 mL	4.277	-0.00961	0.25227	0.00094	12.0 s
44:49.9	Data point 38	1.50000 mL	0.10894 mL	0.11559 mL	0.05000 mL	4.471	-0.01870	0.92262	0.00096	42.5 s
45:57.9	Data point 39	1.50000 mL	0.10894 mL	0.11592 mL	0.05000 mL	4.621	-0.01913	0.96775	0.00096	33.0 s
47:01.5	Data point 40	1.50000 mL	0.10894 mL	0.11637 mL	0.05000 mL	5.064	-0.01981	0.97178	0.00099	36.5 s
48:08.6	Data point 41	1.50000 mL	0.10894 mL	0.11656 mL	0.05000 mL	5.290	-0.01849	0.90940	0.00096	39.5 s
49:18.8	Data point 42	1.50000 mL	0.10894 mL	0.11668 mL	0.05000 mL	5.544	-0.01813	0.90749	0.00094	42.5 s
50:31.9	Data point 43	1.50000 mL	0.10894 mL	0.11684 mL	0.05000 mL	6.152	-0.01812	0.90297	0.00094	54.0 s
51:56.5	Data point 44	1.50000 mL	0.10894 mL	0.11698 mL	0.05000 mL	6.731	-0.03629	0.94871	0.00184	Timed out at 59.5 s
53:32.0	Data point 45	1.50000 mL	0.10894 mL	0.11705 mL	0.05000 mL	6.942	-0.03907	0.98089	0.00195	Timed out at 59.5 s
55:07.6	Data point 46	1.50000 mL	0.10894 mL	0.11717 mL	0.05000 mL	7.360	-0.05485	0.98317	0.00273	Timed out at 59.5 s
56:43.2	Data point 47	1.50000 mL	0.10894 mL	0.11724 mL	0.05000 mL	7.698	-0.06448	0.99495	0.00319	Timed out at 59.5 s
58:18.8	Data point 48	1.50000 mL	0.10894 mL	0.11731 mL	0.05000 mL	7.975	-0.06889	0.99504	0.00341	Timed out at 59.5 s
59:49.3	Data point 49	1.50000 mL	0.10894 mL	0.11736 mL	0.05000 mL	8.218	-0.05194	0.98871	0.00258	Timed out at 59.5 s
1:01:24.9	Data point 50	1.50000 mL	0.10894 mL	0.11743 mL	0.05000 mL	8.279	-0.03256	0.93039	0.00167	Timed out at 59.5 s
1:03:00.6	Data point 51	1.50000 mL	0.10894 mL	0.11764 mL	0.05000 mL	9.044	-0.01889	0.94983	0.00096	35.0 s
1:04:38.7	Data point 52	1.50000 mL	0.17653 mL	0.11764 mL	0.25000 mL	1.983	-0.01328	0.50845	0.00092	10.0 s
1:05:25.0	Data point 53	1.50000 mL	0.17653 mL	0.13808 mL	0.25000 mL	2.188	-0.00421	0.56558	0.00028	10.0 s
1:06:00.8	Data point 54	1.50000 mL	0.17653 mL	0.15059 mL	0.25000 mL	2.379	-0.01117	0.72575	0.00065	10.0 s
1:06:36.4	Data point 55	1.50000 mL	0.17653 mL	0.15924 mL	0.25000 mL	2.563	0.00955	0.39409	0.00075	10.5 s
1:07:12.5	Data point 56	1.50000 mL	0.17653 mL	0.16552 mL	0.25000 mL	2.758	-0.00090	0.01671	0.00034	10.0 s
1:07:48.0	Data point 57	1.50000 mL	0.17653 mL	0.17016 mL	0.25000 mL	2.964	-0.00646	0.68297	0.00039	10.0 s
1:08:23.5	Data point 58	1.50000 mL	0.17653 mL	0.17354 mL	0.25000 mL	3.172	-0.01240	0.57154	0.00081	10.0 s
1:08:59.1	Data point 59	1.50000 mL	0.17653 mL	0.17601 mL	0.25000 mL	3.439	-0.00851	0.81815	0.00046	10.0 s
1:09:39.7	Data point 60	1.50000 mL	0.17653 mL	0.17719 mL	0.25000 mL	3.639	-0.00768	0.92817	0.00039	10.0 s
1:10:20.4	Data point 61	1.50000 mL	0.17653 mL	0.17806 mL	0.25000 mL	3.840	-0.01302	0.73901	0.00075	10.0 s
1:11:06.2	Data point 62	1.50000 mL	0.17653 mL	0.17869 mL	0.25000 mL	4.040	-0.01483	0.68740	0.00088	10.0 s
1:11:41.6	Data point 63	1.50000 mL	0.17653 mL	0.17916 mL	0.25000 mL	4.352	-0.01359	0.79722	0.00075	11.0 s
1:12:23.2	Data point 64	1.50000 mL	0.17653 mL	0.17949 mL	0.25000 mL	4.639	-0.01394	0.58554	0.00090	12.0 s
1:13:05.6	Data point 65	1.50000 mL	0.17653 mL	0.17973 mL	0.25000 mL	4.868	-0.01439	0.70067	0.00085	13.0 s
1:13:54.3	Data point 66	1.50000 mL	0.17653 mL	0.17996 mL	0.25000 mL	5.075	-0.01857	0.88631	0.00097	16.5 s
1:14:46.4	Data point 67	1.50000 mL	0.17653 mL	0.18010 mL	0.25000 mL	5.398	-0.01592	0.73444	0.00092	28.5 s
1:15:45.5	Data point 68	1.50000 mL	0.17653 mL	0.18024 mL	0.25000 mL	5.785	-0.01894	0.91475	0.00098	46.0 s
1:17:02.1	Data point 69	1.50000 mL	0.17653 mL	0.18029 mL	0.25000 mL	6.007	-0.01848	0.84150	0.00100	25.0 s
1:17:52.5	Data point 70	1.50000 mL	0.17653 mL	0.18034 mL	0.25000 mL	6.149	-0.01829	0.90450	0.00095	53.0 s
1:19:21.4	Data point 71	1.50000 mL	0.17653 mL	0.18053 mL	0.25000 mL	6.777	-0.04095	0.98006	0.00204	Timed out at 59.5 s
1:20:57.0	Data point 72	1.50000 mL	0.17653 mL	0.18062 mL	0.25000 mL	7.093	-0.04542	0.98750	0.00225	Timed out at 59.5 s

Sample name: **M12_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03014**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03014_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 6:11:21 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Events (continued)

Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
1:22:32.6	Data point 73	1.50000 mL	0.17653 mL	0.18069 mL	0.25000 mL	7.432	-0.06081	0.97336	0.00305	Timed out at 59.5 s
1:24:08.3	Data point 74	1.50000 mL	0.17653 mL	0.18093 mL	0.25000 mL	8.702	-0.01670	0.95705	0.00084	36.5 s
1:25:20.5	Data point 75	1.50000 mL	0.17653 mL	0.18107 mL	0.25000 mL	8.952	-0.01969	0.97272	0.00099	25.0 s
1:26:21.1	Data point 76	1.50000 mL	0.17653 mL	0.18116 mL	0.25000 mL	9.082	-0.01391	0.60511	0.00088	15.0 s
1:26:45.2	Assay volumes	1.50000 mL	0.17653 mL	0.18116 mL	0.25000 mL					

Sample name: **M12_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03014**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03014_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 6:11:21 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Assay Settings

Setting	Value	Original Value	Date/Time changed	Imported from
General Settings				
Analyst name	Pion			
Standard Experiment Settings				
Number of titrations	3			
Minimum pH	2.000			
Maximum pH	9.000			
pH step between points of	0.200			
Minimum titrant addition	0.00002 mL			
Maximum titrant addition	0.10000 mL			
Argon flow rate	100%			
Start titration using	Cautious pH adjust			
Advanced General Settings				
Detect turbidity using	None			
Collect turbidity sensor data	No			
Collect UV spectra	No			
Stir after titrant addition for	5 seconds			
For titrant addition, stir at	10%			
Titrant Pre-Dose				
Titrant pre-dose	None			
Assay Medium				
ISA water volume	1.50 mL			
Water added	Automatic			
Partition solvent type	Octanol			
Partition volume	0.020 mL			
Partition solvent added	Automatic			
After partition addition, stir for	1 seconds			
Sample Sonication				
Sonicate	Yes			
Adjust pH for sonication	No			
Sonicate for	120 seconds			
After sonication stir for	5 seconds			
Sample Dissolution				
Perform a dissolution stage	Yes			
Adjust and hold pH for dissolution	To start pH			
Stir to dissolve for	120 seconds			
For dissolution, stir at	10%			
Carbonate purge				
Perform a carbonate purge	No			
Temperature Control				
Wait for temperature	Yes			
Required start temperature	25.0°C			
Acceptable deviation	0.5°C			
Time to wait	60 seconds			
Stir speed of	50%			
Titration 1				
Titrate from	Low to high pH			
Adjust to start pH	Yes			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	50%			
Titration 2				
Titrate from	Low to high pH			
Add additional water	0.00 mL			
Additional partition solvent volume	0.030 mL			
Additional partition solvent added	Automatic			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	55%			

Sample name: **M12_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03014**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03014_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 6:11:21 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Assay Settings (continued)

Setting	Value	Original Value	Date/Time changed	Imported from
Titration 3				
Titrate from	Low to high pH			
Add additional water	0.00 mL			
Additional partition solvent volume	0.200 mL			
Additional partition solvent added	Automatic			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	60%			
Data Point Stability				
Stir during data point collection	No			
Delay before data point collection	0 seconds			
Number of points to average	20 points			
Time interval between points	0.50 seconds			
Required maximum standard deviation	0.00100 dpH/dt			
Stability timeout after	60 seconds			

Calibration Settings

Setting	Value	Date/Time changed	Imported from
Four-Plus alpha	0.111	3/3/2018 6:11:21 PM	C:\Sirius_T3\HCl18C02.t3r
Four-Plus S	0.9988	3/3/2018 6:11:21 PM	C:\Sirius_T3\HCl18C02.t3r
Four-Plus jH	1.0	3/3/2018 6:11:21 PM	C:\Sirius_T3\HCl18C02.t3r
Four-Plus jOH	-0.8	3/3/2018 6:11:21 PM	C:\Sirius_T3\HCl18C02.t3r
Base concentration factor	1.000	3/3/2018 6:11:21 PM	C:\Sirius_T3\KOH18B27.t3r
Acid concentration factor	0.999	3/3/2018 6:11:21 PM	C:\Sirius_T3\HCl18C02.t3r

Instrument Settings

Setting	Value	Batch Id	Install date
Instrument owner	Merck		
Instrument ID	T312060		
Instrument type	T3 Simulator		
Software version	1.1.3.0		
Dispenser module		T3DM1200361	3/31/2009 5:24:52 AM
Dispenser 0	Water		3/31/2009 5:25:05 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Water (0.15 M KCl)	02-06-2018	2/27/2018 10:05:59 AM
Dispenser 2	Acid		3/31/2009 5:25:11 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Acid (0.5 M HCl)	02-27-2018	2/27/2018 10:27:22 AM
Dispenser 1	Base		3/31/2009 5:25:21 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Base (0.5 M KOH)	9/22/2017	2/27/2018 10:21:22 AM
Dispenser 5	Cosolvent		3/31/2009 5:26:24 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Distribution valve 5	Distribution Valve		3/31/2009 5:28:19 AM
Firmware version	1.1.3		
Port A	Methanol (80%, 0.15 M KCl)	09-26-17	2/7/2018 9:42:01 AM
Port B	Cyclohexane	11-01-17	2/27/2018 10:37:57 AM
Dispenser 3	Buffer		8/3/2010 5:05:16 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Dodecane	2018/01/31	2/28/2018 10:18:04 AM
Dispenser 6	Octanol		10/22/2010 10:52:43 AM

Sample name: **M12_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03014**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03014_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 6:11:21 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Octanol	01-31-2018	2/27/2018 9:59:35 AM
Titrator		T3TM1200161	3/31/2009 5:24:17 AM
Horizontal axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Probe I/O firmware version	1.1.1		
Electrode	T3 Electrode	T3E0923	1/23/2018 2:01:00 PM
E0 calibration	+6.33 mV		3/3/2018 6:11:49 PM
Filling solution	3M KCl	KCL097	3/2/2018 9:43:24 AM
Liquids			
Wash 1	50% IPA:50% Water		3/2/2018 9:45:12 AM
Wash 2	0.5% Trition X-100 in H20		3/2/2018 9:45:15 AM
Buffer position 1	pH7 Wash		3/2/2018 9:45:18 AM
Buffer position 2	pH 7		3/2/2018 9:45:21 AM
Storage position			3/2/2018 9:44:44 AM
Wash water	6.6e+003 mL	02-27-2018	2/27/2018 9:54:39 AM
Waste	8.9e+003 mL		11/28/2017 10:36:29 AM
Temperature controller			8/5/2010 6:35:13 AM
Turbidity detector			3/31/2009 5:24:45 AM
Spectrometer		074811	11/23/2010 11:22:28 AM
Dip probe		10196	
Wavelength coefficient A0	183.333		
Wavelength coefficient A1	2.21568		
Wavelength coefficient A2	-0.000289308		
Total lamp lit time	120:41:49		11/23/2010 11:22:28 AM
Calibrated on	2/27/2018 10:40:38 AM		
Integration time	40		
Scans averaged	10		
Autoloader		T3AL1200345	11/10/2015 9:34:13 AM
Left-right axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Front-back axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Configuration			
Alternate titration position	Titration position		
Alternate reference position	Reference position		
Maximum standard vial volume	3.50 mL		
Maximum alternate vial volume	25.00 mL		
Automatic action idle period	5 minute(s)		
Titrant tube volume	1.3 mL		
Syringe flush count	3.50		
Flowing wash pump volume	20.0 mL		
Flowing wash stir duration	5 s		
Flowing wash stir speed	30%		
Solvent wash stir duration	5 s		
Solvent wash stir speed	30%		
Surfactant wash stir duration	5 s		
Surfactant wash stir speed	30%		
E0 calibration minimum number of points	10		
E0 calibration maximum standard deviation	0.01500		
E0 calibration timeout period	60 s		
E0 calibration stir duration	5 s		
E0 calibration preparation stir speed	30%		
E0 calibration buffer wash stir duration	5 s		
E0 calibration buffer wash stir speed	30%		
E0 calibration reading stir speed	0%		

Sample name: **M12_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03014**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03014_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 6:11:21 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Spectrometer calibration stir duration	5 s		
Spectrometer calibration stir speed	30%		
Spectrometer calibration wash pump volume	20.0 mL		
Spectrometer calibration wash stir duration	5 s		
Spectrometer calibration wash stir speed	30%		
Overhead dispense height	10000		

Refinement Settings

Setting	Value	Default value
Turbidity detection method	None	None
Turbidity wavelength to assess	500.0 nm	500.0 nm
Turbidity maximum absorbance	0.100	0.100
Turbidity probe threshold	50.00	50.00

Experiment Log

[2:37] Air gap created for Water (0.15 M KCl)
[2:38] Air gap created for Acid (0.5 M HCl)
[2:38] Air gap created for Base (0.5 M KOH)
[2:38] Air gap released for Water (0.15 M KCl)
[2:42] Titrator arm moved over Titration position
[2:42] Titration 1 of 3
[2:42] Adding initial titrants
[2:42] Automatically add 1.50000 mL of water
[3:07] Dispensed 1.500000 mL of Water (0.15 M KCl)
[3:11] Titrator arm moved over Drain
[5:53] Titrator arm moved to Titration position
[5:53] Argon flow rate set to 100
[5:53] Stirrer speed set to 10
[5:58] Automatically add 0.02000 mL of Octanol
[5:58] Dispensed 0.019991 mL of Octanol
[5:59] Initial pH = 3.54
[5:59] Iterative adjust 3.54 -> 2.00
[5:59] pH 3.54 -> 2.00
[6:01] Air gap released for Acid (0.5 M HCl)
[6:02] Dispensed 0.045296 mL of Acid (0.5 M HCl)
[6:07] pH 2.02 -> 2.00
[6:07] Dispensed 0.001552 mL of Acid (0.5 M HCl)
[6:12] Holding pH 2.00
[8:12] Stirrer speed set to 0
[8:12] Stirrer speed set to 50
[8:12] Iterative adjust 1.97 -> 2.00
[8:12] pH 1.97 -> 2.00
[8:13] Air gap released for Base (0.5 M KOH)
[8:14] Dispensed 0.003363 mL of Base (0.5 M KOH)
[9:04] Stirrer speed set to 0
[9:14] Datapoint id 1 collected
[9:14] Stirrer speed set to 50
[9:19] pH 2.04 -> 2.24
[9:19] Using cautious pH adjust
[9:19] Dispensed 0.007079 mL of Base (0.5 M KOH)
[9:24] Stepping pH = 2.12
[9:25] Dispensed 0.006444 mL of Base (0.5 M KOH)
[9:30] Stepping pH = 2.22
[9:30] Dispensed 0.001341 mL of Base (0.5 M KOH)
[9:35] Stepping pH = 2.24
[9:50] Stirrer speed set to 0
[10:01] Datapoint id 2 collected

Sample name: **M12_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03014**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03014_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 6:11:21 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[10:01] Charge balance equation is out by -4.8%
[10:01] Stirrer speed set to 50
[10:06] pH 2.25 -> 2.45
[10:06] Using charge balance adjust
[10:06] Dispensed 0.008984 mL of Base (0.5 M KOH)
[10:26] Stirrer speed set to 0
[10:37] Datapoint id 3 collected
[10:37] Charge balance equation is out by -10.3%
[10:37] Stirrer speed set to 50
[10:42] pH 2.43 -> 2.63
[10:42] Using charge balance adjust
[10:42] Dispensed 0.006115 mL of Base (0.5 M KOH)
[11:02] Stirrer speed set to 0
[11:13] Datapoint id 4 collected
[11:13] Charge balance equation is out by -13.9%
[11:13] Stirrer speed set to 50
[11:18] pH 2.61 -> 2.81
[11:18] Using charge balance adjust
[11:18] Dispensed 0.004398 mL of Base (0.5 M KOH)
[11:38] Stirrer speed set to 0
[11:48] Datapoint id 5 collected
[11:48] Charge balance equation is out by -4.8%
[11:48] Stirrer speed set to 50
[11:54] pH 2.81 -> 3.01
[11:54] Using charge balance adjust
[11:54] Dispensed 0.003316 mL of Base (0.5 M KOH)
[12:14] Stirrer speed set to 0
[12:25] Datapoint id 6 collected
[12:25] Charge balance equation is out by -15.2%
[12:25] Stirrer speed set to 50
[12:30] pH 2.99 -> 3.19
[12:30] Using cautious pH adjust
[12:30] Dispensed 0.001388 mL of Base (0.5 M KOH)
[12:35] Stepping pH = 3.08
[12:35] Dispensed 0.000988 mL of Base (0.5 M KOH)
[12:41] Stepping pH = 3.16
[12:41] Dispensed 0.000259 mL of Base (0.5 M KOH)
[12:46] Stepping pH = 3.18
[13:01] Stirrer speed set to 0
[13:11] Datapoint id 7 collected
[13:11] Charge balance equation is out by 4.7%
[13:11] Stirrer speed set to 50
[13:16] pH 3.16 -> 3.36
[13:16] Using charge balance adjust
[13:17] Dispensed 0.002469 mL of Base (0.5 M KOH)
[13:37] Stirrer speed set to 0
[13:47] Datapoint id 8 collected
[13:47] Charge balance equation is out by 4.1%
[13:47] Stirrer speed set to 50
[13:52] pH 3.37 -> 3.57
[13:52] Using charge balance adjust
[13:52] Dispensed 0.002234 mL of Base (0.5 M KOH)
[14:12] Stirrer speed set to 0
[14:22] Datapoint id 9 collected
[14:22] Charge balance equation is out by -7.1%
[14:22] Stirrer speed set to 50
[14:27] pH 3.56 -> 3.76
[14:27] Using charge balance adjust
[14:28] Dispensed 0.001999 mL of Base (0.5 M KOH)

Sample name: **M12_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03014**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03014_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 6:11:21 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[14:48] Stirrer speed set to 0
[14:58] Datapoint id 10 collected
[14:58] Charge balance equation is out by 13.2%
[14:58] Stirrer speed set to 50
[15:03] pH 3.78 -> 3.98
[15:03] Using charge balance adjust
[15:04] Dispensed 0.001646 mL of Base (0.5 M KOH)
[15:24] Stirrer speed set to 0
[15:53] Datapoint id 11 collected
[15:53] Charge balance equation is out by 42.3%
[15:53] Stirrer speed set to 50
[15:58] pH 4.06 -> 4.26
[15:58] Using cautious pH adjust
[15:59] Dispensed 0.000588 mL of Base (0.5 M KOH)
[16:04] Stepping pH = 4.24
[16:04] Dispensed 0.000047 mL of Base (0.5 M KOH)
[16:09] Stepping pH = 4.21
[16:09] Dispensed 0.000753 mL of Base (0.5 M KOH)
[16:14] Stepping pH = 4.64
[16:29] Stirrer speed set to 0
[16:51] Datapoint id 12 collected
[16:51] Charge balance equation is out by -18.3%
[16:51] Stirrer speed set to 50
[16:56] pH 4.49 -> 4.69
[16:56] Using cautious pH adjust
[16:56] Dispensed 0.000282 mL of Base (0.5 M KOH)
[17:01] Stepping pH = 4.67
[17:01] Dispensed 0.000024 mL of Base (0.5 M KOH)
[17:07] Stepping pH = 4.64
[17:07] Dispensed 0.000306 mL of Base (0.5 M KOH)
[17:12] Stepping pH = 4.98
[17:27] Stirrer speed set to 0
[18:14] Datapoint id 13 collected
[18:14] Charge balance equation is out by -11.2%
[18:14] Stirrer speed set to 50
[18:20] pH 4.89 -> 5.09
[18:20] Using charge balance adjust
[18:20] Dispensed 0.000235 mL of Base (0.5 M KOH)
[18:40] Stirrer speed set to 0
[19:40] Datapoint id 14 collected
[19:40] Charge balance equation is out by -77.2%
[19:40] Stirrer speed set to 50
[19:45] pH 5.03 -> 5.23
[19:45] Using cautious pH adjust
[19:45] Dispensed 0.000094 mL of Base (0.5 M KOH)
[19:50] Stepping pH = 5.04
[19:50] Dispensed 0.000259 mL of Base (0.5 M KOH)
[19:55] Stepping pH = 5.67
[20:10] Stirrer speed set to 0
[21:10] Datapoint id 15 collected
[21:10] Charge balance equation is out by -86.8%
[21:10] Stirrer speed set to 50
[21:16] pH 5.31 -> 5.51
[21:16] Using cautious pH adjust
[21:16] Dispensed 0.000047 mL of Base (0.5 M KOH)
[21:21] Stepping pH = 5.28
[21:21] Dispensed 0.000329 mL of Base (0.5 M KOH)
[21:26] Stepping pH = 6.63
[21:41] Stirrer speed set to 0

Sample name: **M12_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03014**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03014_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 6:11:21 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[22:41] Datapoint id 16 collected
[22:41] Charge balance equation is out by -249.2%
[22:41] Stirrer speed set to 50
[22:46] pH 5.92 -> 6.12
[22:46] Using cautious pH adjust
[22:46] Dispensed 0.000024 mL of Base (0.5 M KOH)
[22:51] Stepping pH = 5.77
[22:51] Dispensed 0.000259 mL of Base (0.5 M KOH)
[22:56] Stepping pH = 6.69
[23:11] Stirrer speed set to 0
[24:11] Datapoint id 17 collected
[24:11] Charge balance equation is out by -408.9%
[24:11] Stirrer speed set to 50
[24:17] pH 5.97 -> 6.17
[24:17] Using cautious pH adjust
[24:17] Dispensed 0.000024 mL of Base (0.5 M KOH)
[24:22] Stepping pH = 5.89
[24:22] Dispensed 0.000212 mL of Base (0.5 M KOH)
[24:27] Stepping pH = 6.77
[24:42] Stirrer speed set to 0
[25:42] Datapoint id 18 collected
[25:42] Charge balance equation is out by -301.9%
[25:42] Stirrer speed set to 50
[25:47] pH 6.27 -> 6.47
[25:47] Using cautious pH adjust
[25:47] Dispensed 0.000024 mL of Base (0.5 M KOH)
[25:52] Stepping pH = 6.23
[25:52] Dispensed 0.000141 mL of Base (0.5 M KOH)
[25:57] Stepping pH = 6.60
[26:12] Stirrer speed set to 0
[27:12] Datapoint id 19 collected
[27:12] Charge balance equation is out by -248.4%
[27:13] Stirrer speed set to 50
[27:18] pH 6.39 -> 6.59
[27:18] Using cautious pH adjust
[27:18] Dispensed 0.000024 mL of Base (0.5 M KOH)
[27:23] Stepping pH = 6.37
[27:23] Dispensed 0.000118 mL of Base (0.5 M KOH)
[27:28] Stepping pH = 6.70
[27:43] Stirrer speed set to 0
[28:43] Datapoint id 20 collected
[28:43] Charge balance equation is out by -226.3%
[28:43] Stirrer speed set to 50
[28:48] pH 6.69 -> 6.89
[28:48] Using cautious pH adjust
[28:48] Dispensed 0.000024 mL of Base (0.5 M KOH)
[28:53] Stepping pH = 6.65
[28:53] Dispensed 0.000094 mL of Base (0.5 M KOH)
[28:58] Stepping pH = 6.93
[29:13] Stirrer speed set to 0
[30:13] Datapoint id 21 collected
[30:13] Charge balance equation is out by -266.6%
[30:13] Stirrer speed set to 50
[30:19] pH 6.92 -> 7.12
[30:19] Using cautious pH adjust
[30:19] Dispensed 0.000024 mL of Base (0.5 M KOH)
[30:24] Stepping pH = 6.85
[30:24] Dispensed 0.000071 mL of Base (0.5 M KOH)
[30:29] Stepping pH = 6.95

Sample name: **M12_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03014**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03014_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 6:11:21 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[30:29] Dispensed 0.000071 mL of Base (0.5 M KOH)
[30:34] Stepping pH = 7.36
[30:49] Stirrer speed set to 0
[31:49] Datapoint id 22 collected
[31:49] Charge balance equation is out by -694.1%
[31:49] Stirrer speed set to 50
[31:54] pH 7.29 -> 7.49
[31:54] Using cautious pH adjust
[31:54] Dispensed 0.000024 mL of Base (0.5 M KOH)
[31:59] Stepping pH = 7.25
[31:59] Dispensed 0.000024 mL of Base (0.5 M KOH)
[32:05] Stepping pH = 7.22
[32:05] Dispensed 0.000188 mL of Base (0.5 M KOH)
[32:10] Stepping pH = 8.57
[32:25] Stirrer speed set to 0
[33:25] Datapoint id 23 collected
[33:25] Charge balance equation is out by -2,178.7%
[33:25] Stirrer speed set to 50
[33:30] pH 8.80 -> 9.00
[33:30] Using cautious pH adjust
[33:30] Dispensed 0.000024 mL of Base (0.5 M KOH)
[33:35] Stepping pH = 8.79
[33:35] Dispensed 0.000071 mL of Base (0.5 M KOH)
[33:40] Stepping pH = 8.89
[33:40] Dispensed 0.000071 mL of Base (0.5 M KOH)
[33:45] Stepping pH = 9.02
[34:00] Stirrer speed set to 0
[35:00] Datapoint id 24 collected
[35:01] Charge balance equation is out by -456.4%
[35:01] Stirrer speed set to 50
[35:06] pH 8.94 -> 9.05
[35:06] Using cautious pH adjust
[35:06] Dispensed 0.000024 mL of Base (0.5 M KOH)
[35:11] Stepping pH = 8.91
[35:11] Dispensed 0.000047 mL of Base (0.5 M KOH)
[35:16] Stepping pH = 8.96
[35:16] Dispensed 0.000047 mL of Base (0.5 M KOH)
[35:21] Stepping pH = 9.16
[35:36] Stirrer speed set to 0
[36:24] Datapoint id 25 collected
[36:24] Charge balance equation is out by -631.2%
[36:24] Titration 2 of 3
[36:24] Adding initial titrants
[36:24] Automatically add 0.03000 mL of Octanol
[36:25] Dispensed 0.030009 mL of Octanol
[36:25] Stirrer speed set to 10
[36:26] Stirrer speed set to 55
[36:26] Iterative adjust 9.17 -> 2.00
[36:26] pH 9.17 -> 2.00
[36:28] Dispensed 0.056138 mL of Acid (0.5 M HCl)
[36:33] pH 2.05 -> 2.00
[36:33] Dispensed 0.004633 mL of Acid (0.5 M HCl)
[36:38] pH 2.01 -> 2.00
[36:38] Dispensed 0.001317 mL of Acid (0.5 M HCl)
[37:28] Stirrer speed set to 0
[37:38] Datapoint id 26 collected
[37:38] Stirrer speed set to 55
[37:43] pH 1.99 -> 2.19
[37:43] Using cautious pH adjust

Sample name: **M12_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03014**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03014_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 6:11:21 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[37:44] Dispensed 0.008725 mL of Base (0.5 M KOH)
[37:49] Stepping pH = 2.07
[37:49] Dispensed 0.007079 mL of Base (0.5 M KOH)
[37:54] Stepping pH = 2.15
[37:54] Dispensed 0.002611 mL of Base (0.5 M KOH)
[38:00] Stepping pH = 2.19
[38:15] Stirrer speed set to 0
[38:25] Datapoint id 27 collected
[38:25] Charge balance equation is out by -5.5%
[38:25] Stirrer speed set to 55
[38:30] pH 2.19 -> 2.39
[38:30] Using charge balance adjust
[38:31] Dispensed 0.011218 mL of Base (0.5 M KOH)
[38:51] Stirrer speed set to 0
[39:01] Datapoint id 28 collected
[39:01] Charge balance equation is out by -2.0%
[39:01] Stirrer speed set to 55
[39:06] pH 2.39 -> 2.59
[39:06] Using charge balance adjust
[39:06] Dispensed 0.007479 mL of Base (0.5 M KOH)
[39:26] Stirrer speed set to 0
[39:36] Datapoint id 29 collected
[39:36] Charge balance equation is out by -11.7%
[39:36] Stirrer speed set to 55
[39:41] pH 2.57 -> 2.77
[39:41] Using charge balance adjust
[39:42] Dispensed 0.005409 mL of Base (0.5 M KOH)
[40:02] Stirrer speed set to 0
[40:12] Datapoint id 30 collected
[40:12] Charge balance equation is out by -10.8%
[40:12] Stirrer speed set to 55
[40:17] pH 2.76 -> 2.96
[40:17] Using charge balance adjust
[40:18] Dispensed 0.004163 mL of Base (0.5 M KOH)
[40:38] Stirrer speed set to 0
[40:48] Datapoint id 31 collected
[40:48] Charge balance equation is out by 7.0%
[40:48] Stirrer speed set to 55
[40:53] pH 2.97 -> 3.17
[40:53] Using charge balance adjust
[40:53] Dispensed 0.003269 mL of Base (0.5 M KOH)
[41:13] Stirrer speed set to 0
[41:24] Datapoint id 32 collected
[41:24] Charge balance equation is out by -9.7%
[41:24] Stirrer speed set to 55
[41:29] pH 3.15 -> 3.35
[41:29] Using charge balance adjust
[41:29] Dispensed 0.002752 mL of Base (0.5 M KOH)
[41:49] Stirrer speed set to 0
[41:59] Datapoint id 33 collected
[41:59] Charge balance equation is out by 8.4%
[41:59] Stirrer speed set to 55
[42:04] pH 3.37 -> 3.57
[42:04] Using charge balance adjust
[42:04] Dispensed 0.002187 mL of Base (0.5 M KOH)
[42:24] Stirrer speed set to 0
[42:34] Datapoint id 34 collected
[42:34] Charge balance equation is out by 10.6%
[42:34] Stirrer speed set to 55

Sample name: **M12_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03014**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03014_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 6:11:21 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[42:40] pH 3.60 -> 3.80
[42:40] Using charge balance adjust
[42:40] Dispensed 0.001646 mL of Base (0.5 M KOH)
[43:00] Stirrer speed set to 0
[43:10] Datapoint id 35 collected
[43:10] Charge balance equation is out by 11.7%
[43:10] Stirrer speed set to 55
[43:16] pH 3.83 -> 4.03
[43:16] Using charge balance adjust
[43:16] Dispensed 0.001176 mL of Base (0.5 M KOH)
[43:36] Stirrer speed set to 0
[43:47] Datapoint id 36 collected
[43:47] Charge balance equation is out by 6.6%
[43:47] Stirrer speed set to 55
[43:52] pH 4.06 -> 4.26
[43:52] Using charge balance adjust
[43:52] Dispensed 0.000776 mL of Base (0.5 M KOH)
[44:12] Stirrer speed set to 0
[44:24] Datapoint id 37 collected
[44:24] Charge balance equation is out by 10.2%
[44:24] Stirrer speed set to 55
[44:29] pH 4.29 -> 4.49
[44:29] Using charge balance adjust
[44:29] Dispensed 0.000494 mL of Base (0.5 M KOH)
[44:50] Stirrer speed set to 0
[45:32] Datapoint id 38 collected
[45:32] Charge balance equation is out by -11.9%
[45:32] Stirrer speed set to 55
[45:37] pH 4.50 -> 4.70
[45:37] Using charge balance adjust
[45:37] Dispensed 0.000329 mL of Base (0.5 M KOH)
[45:58] Stirrer speed set to 0
[46:31] Datapoint id 39 collected
[46:31] Charge balance equation is out by -38.3%
[46:31] Stirrer speed set to 55
[46:36] pH 4.65 -> 4.85
[46:36] Using cautious pH adjust
[46:36] Dispensed 0.000118 mL of Base (0.5 M KOH)
[46:41] Stepping pH = 4.66
[46:41] Dispensed 0.000329 mL of Base (0.5 M KOH)
[46:46] Stepping pH = 5.18
[47:01] Stirrer speed set to 0
[47:38] Datapoint id 40 collected
[47:38] Charge balance equation is out by -91.6%
[47:38] Stirrer speed set to 55
[47:43] pH 5.10 -> 5.30
[47:43] Using cautious pH adjust
[47:43] Dispensed 0.000047 mL of Base (0.5 M KOH)
[47:48] Stepping pH = 5.11
[47:48] Dispensed 0.000141 mL of Base (0.5 M KOH)
[47:53] Stepping pH = 5.38
[48:08] Stirrer speed set to 0
[48:48] Datapoint id 41 collected
[48:48] Charge balance equation is out by -92.4%
[48:48] Stirrer speed set to 55
[48:53] pH 5.32 -> 5.52
[48:53] Using cautious pH adjust
[48:53] Dispensed 0.000024 mL of Base (0.5 M KOH)
[48:58] Stepping pH = 5.34

Sample name: **M12_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03014**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03014_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 6:11:21 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[48:58] Dispensed 0.000094 mL of Base (0.5 M KOH)
[49:03] Stepping pH = 5.61
[49:19] Stirrer speed set to 0
[50:01] Datapoint id 42 collected
[50:01] Charge balance equation is out by -86.2%
[50:01] Stirrer speed set to 55
[50:06] pH 5.58 -> 5.78
[50:06] Using cautious pH adjust
[50:06] Dispensed 0.000024 mL of Base (0.5 M KOH)
[50:11] Stepping pH = 5.58
[50:11] Dispensed 0.000141 mL of Base (0.5 M KOH)
[50:17] Stepping pH = 6.15
[50:32] Stirrer speed set to 0
[51:26] Datapoint id 43 collected
[51:26] Charge balance equation is out by -209.7%
[51:26] Stirrer speed set to 55
[51:31] pH 6.15 -> 6.35
[51:31] Using cautious pH adjust
[51:31] Dispensed 0.000024 mL of Base (0.5 M KOH)
[51:36] Stepping pH = 6.15
[51:36] Dispensed 0.000118 mL of Base (0.5 M KOH)
[51:41] Stepping pH = 6.66
[51:56] Stirrer speed set to 0
[52:56] Datapoint id 44 collected
[52:56] Charge balance equation is out by -201.5%
[52:56] Stirrer speed set to 55
[53:01] pH 6.73 -> 6.93
[53:01] Using cautious pH adjust
[53:01] Dispensed 0.000024 mL of Base (0.5 M KOH)
[53:06] Stepping pH = 6.77
[53:06] Dispensed 0.000024 mL of Base (0.5 M KOH)
[53:12] Stepping pH = 6.86
[53:12] Dispensed 0.000024 mL of Base (0.5 M KOH)
[53:17] Stepping pH = 6.98
[53:32] Stirrer speed set to 0
[54:32] Datapoint id 45 collected
[54:32] Charge balance equation is out by -131.1%
[54:32] Stirrer speed set to 55
[54:37] pH 6.91 -> 7.11
[54:37] Using cautious pH adjust
[54:37] Dispensed 0.000024 mL of Base (0.5 M KOH)
[54:42] Stepping pH = 6.88
[54:42] Dispensed 0.000071 mL of Base (0.5 M KOH)
[54:47] Stepping pH = 7.09
[54:47] Dispensed 0.000024 mL of Base (0.5 M KOH)
[54:52] Stepping pH = 7.32
[55:07] Stirrer speed set to 0
[56:07] Datapoint id 46 collected
[56:07] Charge balance equation is out by -381.0%
[56:07] Stirrer speed set to 55
[56:13] pH 7.34 -> 7.54
[56:13] Using cautious pH adjust
[56:13] Dispensed 0.000024 mL of Base (0.5 M KOH)
[56:18] Stepping pH = 7.34
[56:18] Dispensed 0.000024 mL of Base (0.5 M KOH)
[56:23] Stepping pH = 7.41
[56:23] Dispensed 0.000024 mL of Base (0.5 M KOH)
[56:28] Stepping pH = 7.58
[56:43] Stirrer speed set to 0

Sample name: **M12_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03014**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03014_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 6:11:21 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[57:43] Datapoint id 47 collected
[57:43] Charge balance equation is out by -592.2%
[57:43] Stirrer speed set to 55
[57:48] pH 7.62 -> 7.82
[57:48] Using cautious pH adjust
[57:48] Dispensed 0.000024 mL of Base (0.5 M KOH)
[57:53] Stepping pH = 7.57
[57:53] Dispensed 0.000024 mL of Base (0.5 M KOH)
[57:58] Stepping pH = 7.67
[57:58] Dispensed 0.000024 mL of Base (0.5 M KOH)
[58:04] Stepping pH = 7.88
[58:19] Stirrer speed set to 0
[59:19] Datapoint id 48 collected
[59:19] Charge balance equation is out by -780.6%
[59:19] Stirrer speed set to 55
[59:24] pH 7.95 -> 8.15
[59:24] Using cautious pH adjust
[59:24] Dispensed 0.000024 mL of Base (0.5 M KOH)
[59:29] Stepping pH = 8.00
[59:29] Dispensed 0.000024 mL of Base (0.5 M KOH)
[59:34] Stepping pH = 8.15
[59:49] Stirrer speed set to 0
[1:00:49] Datapoint id 49 collected
[1:00:49] Charge balance equation is out by -477.9%
[1:00:49] Stirrer speed set to 55
[1:00:54] pH 8.16 -> 8.36
[1:00:54] Using cautious pH adjust
[1:00:54] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:00:59] Stepping pH = 8.15
[1:00:59] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:01:04] Stepping pH = 8.21
[1:01:05] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:01:10] Stepping pH = 8.35
[1:01:25] Stirrer speed set to 0
[1:02:25] Datapoint id 50 collected
[1:02:25] Charge balance equation is out by -765.8%
[1:02:25] Stirrer speed set to 55
[1:02:30] pH 8.21 -> 8.41
[1:02:30] Using cautious pH adjust
[1:02:30] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:02:35] Stepping pH = 8.16
[1:02:35] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:02:40] Stepping pH = 8.12
[1:02:40] Dispensed 0.000165 mL of Base (0.5 M KOH)
[1:02:45] Stepping pH = 8.99
[1:03:00] Stirrer speed set to 0
[1:03:35] Datapoint id 51 collected
[1:03:35] Charge balance equation is out by -2,119.2%
[1:03:35] Titration 3 of 3
[1:03:35] Adding initial titrants
[1:03:35] Automatically add 0.20000 mL of Octanol
[1:03:40] Dispensed 0.200000 mL of Octanol
[1:03:40] Stirrer speed set to 10
[1:03:41] Stirrer speed set to 60
[1:03:41] Iterative adjust 9.05 -> 2.00
[1:03:41] pH 9.05 -> 2.00
[1:03:43] Dispensed 0.058467 mL of Acid (0.5 M HCl)
[1:03:48] pH 2.09 -> 2.00
[1:03:48] Dispensed 0.009125 mL of Acid (0.5 M HCl)

Sample name: **M12_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03014**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03014_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 6:11:21 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[1:04:38] Stirrer speed set to 0
[1:04:48] Datapoint id 52 collected
[1:04:48] Stirrer speed set to 60
[1:04:54] pH 1.99 -> 2.19
[1:04:54] Using cautious pH adjust
[1:04:54] Dispensed 0.009548 mL of Base (0.5 M KOH)
[1:04:59] Stepping pH = 2.07
[1:04:59] Dispensed 0.007973 mL of Base (0.5 M KOH)
[1:05:04] Stepping pH = 2.15
[1:05:05] Dispensed 0.002916 mL of Base (0.5 M KOH)
[1:05:10] Stepping pH = 2.19
[1:05:25] Stirrer speed set to 0
[1:05:35] Datapoint id 53 collected
[1:05:35] Charge balance equation is out by -7.1%
[1:05:35] Stirrer speed set to 60
[1:05:40] pH 2.19 -> 2.39
[1:05:40] Using charge balance adjust
[1:05:40] Dispensed 0.012512 mL of Base (0.5 M KOH)
[1:06:01] Stirrer speed set to 0
[1:06:11] Datapoint id 54 collected
[1:06:11] Charge balance equation is out by -6.0%
[1:06:11] Stirrer speed set to 60
[1:06:16] pH 2.38 -> 2.58
[1:06:16] Using charge balance adjust
[1:06:16] Dispensed 0.008655 mL of Base (0.5 M KOH)
[1:06:36] Stirrer speed set to 0
[1:06:47] Datapoint id 55 collected
[1:06:47] Charge balance equation is out by -9.8%
[1:06:47] Stirrer speed set to 60
[1:06:52] pH 2.57 -> 2.77
[1:06:52] Using charge balance adjust
[1:06:52] Dispensed 0.006279 mL of Base (0.5 M KOH)
[1:07:12] Stirrer speed set to 0
[1:07:22] Datapoint id 56 collected
[1:07:22] Charge balance equation is out by -5.8%
[1:07:22] Stirrer speed set to 60
[1:07:27] pH 2.76 -> 2.96
[1:07:27] Using charge balance adjust
[1:07:28] Dispensed 0.004633 mL of Base (0.5 M KOH)
[1:07:48] Stirrer speed set to 0
[1:07:58] Datapoint id 57 collected
[1:07:58] Charge balance equation is out by 0.1%
[1:07:58] Stirrer speed set to 60
[1:08:03] pH 2.97 -> 3.17
[1:08:03] Using charge balance adjust
[1:08:03] Dispensed 0.003387 mL of Base (0.5 M KOH)
[1:08:23] Stirrer speed set to 0
[1:08:33] Datapoint id 58 collected
[1:08:33] Charge balance equation is out by 0.6%
[1:08:33] Stirrer speed set to 60
[1:08:38] pH 3.18 -> 3.38
[1:08:38] Using charge balance adjust
[1:08:39] Dispensed 0.002469 mL of Base (0.5 M KOH)
[1:08:59] Stirrer speed set to 0
[1:09:09] Datapoint id 59 collected
[1:09:09] Charge balance equation is out by 31.4%
[1:09:09] Stirrer speed set to 60
[1:09:14] pH 3.45 -> 3.65
[1:09:14] Using cautious pH adjust

Sample name: **M12_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03014**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03014_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 6:11:21 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[1:09:14] Dispensed 0.000776 mL of Base (0.5 M KOH)
[1:09:19] Stepping pH = 3.56
[1:09:19] Dispensed 0.000400 mL of Base (0.5 M KOH)
[1:09:24] Stepping pH = 3.64
[1:09:39] Stirrer speed set to 0
[1:09:49] Datapoint id 60 collected
[1:09:49] Charge balance equation is out by 23.3%
[1:09:49] Stirrer speed set to 60
[1:09:55] pH 3.65 -> 3.85
[1:09:55] Using cautious pH adjust
[1:09:55] Dispensed 0.000517 mL of Base (0.5 M KOH)
[1:10:00] Stepping pH = 3.74
[1:10:00] Dispensed 0.000353 mL of Base (0.5 M KOH)
[1:10:05] Stepping pH = 3.84
[1:10:20] Stirrer speed set to 0
[1:10:30] Datapoint id 61 collected
[1:10:30] Charge balance equation is out by 16.0%
[1:10:30] Stirrer speed set to 60
[1:10:35] pH 3.85 -> 4.05
[1:10:35] Using cautious pH adjust
[1:10:35] Dispensed 0.000353 mL of Base (0.5 M KOH)
[1:10:41] Stepping pH = 3.95
[1:10:41] Dispensed 0.000235 mL of Base (0.5 M KOH)
[1:10:46] Stepping pH = 4.03
[1:10:46] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:10:51] Stepping pH = 4.04
[1:11:06] Stirrer speed set to 0
[1:11:16] Datapoint id 62 collected
[1:11:16] Charge balance equation is out by 12.2%
[1:11:16] Stirrer speed set to 60
[1:11:21] pH 4.05 -> 4.25
[1:11:21] Using charge balance adjust
[1:11:21] Dispensed 0.000470 mL of Base (0.5 M KOH)
[1:11:41] Stirrer speed set to 0
[1:11:52] Datapoint id 63 collected
[1:11:52] Charge balance equation is out by 53.3%
[1:11:52] Stirrer speed set to 60
[1:11:57] pH 4.37 -> 4.57
[1:11:57] Using cautious pH adjust
[1:11:58] Dispensed 0.000118 mL of Base (0.5 M KOH)
[1:12:03] Stepping pH = 4.40
[1:12:03] Dispensed 0.000212 mL of Base (0.5 M KOH)
[1:12:08] Stepping pH = 4.63
[1:12:23] Stirrer speed set to 0
[1:12:35] Datapoint id 64 collected
[1:12:35] Charge balance equation is out by -42.4%
[1:12:35] Stirrer speed set to 60
[1:12:40] pH 4.66 -> 4.86
[1:12:40] Using cautious pH adjust
[1:12:40] Dispensed 0.000071 mL of Base (0.5 M KOH)
[1:12:45] Stepping pH = 4.68
[1:12:45] Dispensed 0.000165 mL of Base (0.5 M KOH)
[1:12:50] Stepping pH = 4.86
[1:13:05] Stirrer speed set to 0
[1:13:18] Datapoint id 65 collected
[1:13:18] Charge balance equation is out by -88.6%
[1:13:18] Stirrer speed set to 60
[1:13:23] pH 4.89 -> 5.09
[1:13:24] Using cautious pH adjust

Sample name: **M12_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03014**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03014_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 6:11:21 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[1:13:24] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:13:29] Stepping pH = 4.90
[1:13:29] Dispensed 0.000118 mL of Base (0.5 M KOH)
[1:13:34] Stepping pH = 4.99
[1:13:34] Dispensed 0.000071 mL of Base (0.5 M KOH)
[1:13:39] Stepping pH = 5.09
[1:13:54] Stirrer speed set to 0
[1:14:11] Datapoint id 66 collected
[1:14:11] Charge balance equation is out by -190.1%
[1:14:11] Stirrer speed set to 60
[1:14:16] pH 5.10 -> 5.30
[1:14:16] Using cautious pH adjust
[1:14:16] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:14:21] Stepping pH = 5.11
[1:14:21] Dispensed 0.000071 mL of Base (0.5 M KOH)
[1:14:26] Stepping pH = 5.22
[1:14:26] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:14:31] Stepping pH = 5.38
[1:14:46] Stirrer speed set to 0
[1:15:15] Datapoint id 67 collected
[1:15:15] Charge balance equation is out by -164.6%
[1:15:15] Stirrer speed set to 60
[1:15:20] pH 5.41 -> 5.61
[1:15:20] Using cautious pH adjust
[1:15:20] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:15:25] Stepping pH = 5.39
[1:15:25] Dispensed 0.000118 mL of Base (0.5 M KOH)
[1:15:30] Stepping pH = 5.71
[1:15:45] Stirrer speed set to 0
[1:16:31] Datapoint id 68 collected
[1:16:31] Charge balance equation is out by -225.5%
[1:16:31] Stirrer speed set to 60
[1:16:36] pH 5.83 -> 6.03
[1:16:36] Using cautious pH adjust
[1:16:36] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:16:42] Stepping pH = 5.89
[1:16:42] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:16:47] Stepping pH = 6.03
[1:17:02] Stirrer speed set to 0
[1:17:27] Datapoint id 69 collected
[1:17:27] Charge balance equation is out by -8.4%
[1:17:27] Stirrer speed set to 60
[1:17:32] pH 5.99 -> 6.19
[1:17:32] Using charge balance adjust
[1:17:32] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:17:52] Stirrer speed set to 0
[1:18:45] Datapoint id 70 collected
[1:18:45] Charge balance equation is out by -19.7%
[1:18:45] Stirrer speed set to 60
[1:18:50] pH 6.13 -> 6.33
[1:18:50] Using cautious pH adjust
[1:18:50] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:18:56] Stepping pH = 6.13
[1:18:56] Dispensed 0.000071 mL of Base (0.5 M KOH)
[1:19:01] Stepping pH = 6.19
[1:19:01] Dispensed 0.000094 mL of Base (0.5 M KOH)
[1:19:06] Stepping pH = 6.80
[1:19:21] Stirrer speed set to 0
[1:20:21] Datapoint id 71 collected

Sample name: **M12_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03014**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03014_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 6:11:21 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[1:20:21] Charge balance equation is out by -288.0%
[1:20:21] Stirrer speed set to 60
[1:20:26] pH 6.74 -> 6.94
[1:20:26] Using cautious pH adjust
[1:20:26] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:20:31] Stepping pH = 6.75
[1:20:31] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:20:37] Stepping pH = 6.90
[1:20:37] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:20:42] Stepping pH = 7.06
[1:20:57] Stirrer speed set to 0
[1:21:57] Datapoint id 72 collected
[1:21:57] Charge balance equation is out by -166.3%
[1:21:57] Stirrer speed set to 60
[1:22:02] pH 7.10 -> 7.30
[1:22:02] Using cautious pH adjust
[1:22:02] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:22:07] Stepping pH = 7.14
[1:22:07] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:22:12] Stepping pH = 7.26
[1:22:12] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:22:17] Stepping pH = 7.42
[1:22:32] Stirrer speed set to 0
[1:23:32] Datapoint id 73 collected
[1:23:32] Charge balance equation is out by -199.6%
[1:23:32] Stirrer speed set to 60
[1:23:37] pH 7.39 -> 7.59
[1:23:37] Using cautious pH adjust
[1:23:38] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:23:43] Stepping pH = 7.37
[1:23:43] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:23:48] Stepping pH = 7.35
[1:23:48] Dispensed 0.000188 mL of Base (0.5 M KOH)
[1:23:53] Stepping pH = 8.65
[1:24:08] Stirrer speed set to 0
[1:24:45] Datapoint id 74 collected
[1:24:45] Charge balance equation is out by -1,860.7%
[1:24:45] Stirrer speed set to 60
[1:24:50] pH 8.76 -> 8.96
[1:24:50] Using cautious pH adjust
[1:24:50] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:24:55] Stepping pH = 8.76
[1:24:55] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:25:00] Stepping pH = 8.82
[1:25:00] Dispensed 0.000071 mL of Base (0.5 M KOH)
[1:25:05] Stepping pH = 8.95
[1:25:20] Stirrer speed set to 0
[1:25:45] Datapoint id 75 collected
[1:25:45] Charge balance equation is out by -332.5%
[1:25:45] Stirrer speed set to 60
[1:25:50] pH 8.97 -> 9.05
[1:25:50] Using cautious pH adjust
[1:25:50] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:25:56] Stepping pH = 8.99
[1:25:56] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:26:01] Stepping pH = 8.99
[1:26:01] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:26:06] Stepping pH = 9.08
[1:26:21] Stirrer speed set to 0

Sample name:	**M12_octanol**	Experiment start time:	**3/3/2018 6:11:21 PM**
Assay name:	**pH-metric high logP**	Analyst:	**Pion**
Assay ID:	**18C-03014**	Instrument ID:	**T312060**
Filename:	**C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03014_M12_octanol_pH-metric high logP.t3r**		

Experiment Log (continued)

[1:26:36] Datapoint id 76 collected
[1:26:36] Charge balance equation is out by -438.5%
[1:26:36] Argon flow rate set to 0
[1:26:40] Titrator arm moved over Titration position